AD-A106 077 KAMAN TEMPO SANTA BARBARA CA F/G 4/1

THE ROSCOE MANUAL. VOLUME 28-1. MOLECULAR BAND MODEL PARAMETERS--ETC(U)

JAN 81 T L STEPHENS, A L KLEIN DNA001-80-C-0030

UNCLASSIFIED KT-81-002(R)-VOL-28-1 DNA-3964F-28-1 NL

1 OF 1

AD A
106077

END

DATE FILMED

11-81

DTIC

(12)

DNA 3964F-28-1

AD A106077

THE ROSCOE MANUAL

Volume 28-1-Molecular Band Model Parameters For Thermal Emissions: Expanded Wavelength Coverage

Kaman Tempo
816 State Street (P.O. Drawer QQ)
Santa Barbara, California 93102

31 January 1981

Final Report for Period 9 November 1979—31 January 1981

CONTRACT No. DNA 001-80-C-0030

DTIC FILE COPY

APPROVED FOR PUBLIC RELEASE;
DISTRIBUTION UNLIMITED.

THIS WORK SPONSORED BY THE DEFENSE NUCLEAR AGENCY UNDER RDT&E RMSS CODES B322080464 S99QAXHC30104 H2590D AND X322080469 Q26QAXHC30101 H2590D.

Prepared for
Director
DEFENSE NUCLEAR AGENCY
Washington, D. C. 20305

81 10 23

REPORT DOCUMENTATION PAGE

READ INSTRUCTIONS BEFORE COMPLETING FORM

1. REPORT NUMBER
DNA 3964F-28-1

2. GOVT ACCESSION NO.
AD-A106 077

3. RECIPIENT'S CATALOG NUMBER

4. TITLE (and Subtitle)
THE ROSCOE MANUAL.
Volume 28-1. Molecular Band Model Parameters for Thermal Emissions: Expanded Wavelength Coverage

5. TYPE OF REPORT & PERIOD COVERED
Final Rep[redacted]t. ~~for Period~~
9 Nov 79 — 31 Jan 81

6. PERFORMING ORG. REPORT NUMBER
KT-81-002(R)

7. AUTHOR(s)
Timothy L. Stephens
Alice L. Klein

8. CONTRACT OR GRANT NUMBER(s)
DNA 001-80-C-0030

9. PERFORMING ORGANIZATION NAME AND ADDRESS
Kaman Tempo
816 State Street (P.O. Drawer QQ)
Santa Barbara, California 93102

10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
Subtasks S99QAXHC301-04
Q26QAXHC301-01

11. CONTROLLING OFFICE NAME AND ADDRESS
Director
Defense Nuclear Agency
Washington, DC 20305

12. REPORT DATE
31 Jan[redacted]81

13. NUMBER OF PAGES
54

14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)

15. SECURITY CLASS. (of this report)
UNCLASSIFIED

15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
N/A

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

This work sponsored by the Defense Nuclear Agency under RTD&E RMSS Codes B322080464 S99QAXHC30104 H2590D and X322080469 Q26QAXHC30101 H2590D.

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Band Model	Nitrous Oxide	Carbon Monoxide	Metal Oxides
Infrared	Nitrogen Dioxide	Methane	ROSCOE Code
Absorption	Ozone	Water Vapor	
Nitric Oxide	Carbon Dioxide	Hydroxyl	

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

The spectral range of band model parameters for the ROSCOE thermal emission has been extended to cover the 2- to 100-micron region. Sources for the new parameter compilation are documented, and graphical representations of the parameters at selected temperatures are presented.

UNCLASSIFIED
SECURITY CLASSIFICATION OF THIS PAGE(When Data Entered)

UNCLASSIFIED
SECURITY CLASSIFICATION OF THIS PAGE(When Data Entered)

TABLE OF CONTENTS

LIST OF ILLUSTRATIONS

List of Illustrations (cont'd)

SECTION 1
INTRODUCTION

The molecular thermal emission model in ROSCOE is documented in Volume 28, *Molecular Band Models for Thermal and Optically Pumped Emissions.* Thermal emissions arise under conditions of local thermodynamic equilibrium (LTE). These conditions occur when collisions are sufficiently frequent to maintain equilibrium. The use of Kirchhoff's law to obtain emission from absorption, which applies in this situation, is discussed in Volume 31, *Sight Path Integration.*

The original model covered only the 2- to 5-micron region (SWIR). The present work expands the data base used by the model to LWIR wavelengths. Band model parameters are now provided for the 2- to 100-micron spectral range. In addition parameters for metal oxides have been added and parameters for certain other molecules have been upgraded.

Section 2 documents the sources used for the revised parameter set as a function of species, wavelength and temperature. In addition the weak line and strong line parameters (describing absorption in optically thin and thick regions respectively) are shown graphically at temperatures of 300 and 3000 K.

SECTION 2
LTE MOLECULAR BAND SHAPES

MODEL IMPLEMENTATION IN ROSCOE

The ROSCOE model for LTE (local thermodynamic equilibrium) molecular band emission and absorption is documented in Reference 2-1. In its original form the model was developed only for the SWIR spectral region between 2000 and 5000 cm^{-1} (2 to 5 microns). In the present effort, the spectral coverage of the model was extended to the LWIR. This was accomplished primarily by augmenting the data base containing weak line and strong line parameters for the molecular species of interest.

The revised data tape contains parameters for the species listed in Table 2-1. The spectral coverage now extends from 100 to 5000 cm^{-1} (2 to 100 microns). The data base, however, does not contain contributions from pure rotational bands of several species, which are important at wavelengths beyond 25 microns. (The pure rotational contributions of H_2O are included in the data base; these are important at wavelengths shorter than 25 microns.) Therefore, the revised data base can be used with confidence in the wavelength region between 2 and 25 microns. Other aspects of the data tape, such as the 5 cm^{-1} wave number resolution and the 200 to 7000 K temperature coverage, remain unchanged from Reference 2-1.

Although band model parameters have been provided for 19 species in the new data set, thermal emission and absorption in ROSCOE are still calculated only for the 10 species originally included in the code (denoted by "a" in the last column of Table 2-1). Since the parameters for other species (primarily metal oxides) were available on the WOE II data tape (Reference 2-2), they were incorporated into ROSCOE for use at a future time when concentrations of these additional species may be calculated.

The Lorentz half-width for pressure-broadened molecular lines is required by the ROSCOE LTE band model. The Lorentz half-width used in the revised model, $\alpha_L^i(STP)$ on page 12 of Reference 2-1, can be determined from Table 2-1 according to the relation

$$\alpha_L^i(STP) = \alpha_L^i(T_{ref}) \sqrt{T_{ref}/273} \quad . \qquad (2-1)$$

Values for $\alpha_L^i(T_{ref})$ and T_{ref} are given in Table 2-1.

MOLECULAR BAND SHAPE PARAMETERS

The development of the molecular band shape parameter data set used in the revised ROSCOE model has been described in Section 6 of Reference 2-2. Table 2-2, taken from Reference 2-2, summarizes the sources of data used in the model.

The revised parameters generated according to the procedure described in Reference 2-2 have not been previously published. Graphical representations of these parameters at two selected temperatures (300 and 3000 K) are therefore included

Table 2-1. Lorentz half-width parameters.

Species	$\alpha_L^i(T_{ref})$	T_{ref}	Source (See Notes)
AℓO	0.04	300	b
CH_4	0.06	273	a
CO	0.06	273	a
CO_2	0.07	273	a
CuO	0.04	300	b
FeO	0.04	300	b
H_2O	0.04	273	a
HNO_3	0.05	273	c
LiO	0.04	300	b
MgO	0.04	300	b
NO	0.04	273	a
NO^+	0.04	273	a
N_2O	0.08	273	a
NO_2	0.10	273	a
OH	0.06	273	a
O_3	0.11	273	a
SiO	0.04	300	b
TiO	0.04	300	b
UO	0.04	300	b

Notes:

[a]Unchanged from Reference 2-1.

[b]See Section 5 of Reference 2-3.

[c]Reference 2-4.

as Figures 2-1 to 2-38. The data compilation consists of the two parameters,

- SOD, the average line strength
- DEI, the reciprocal of the effective line spacing,

which are defined explicitly in Equations 2-7 and 2-8 of Reference 2-1.

Figures 2-1 through 2-38 show the weak line parameters

SOD

and the strong line parameters

Table 2-2. Sources of LTE band shape data.

Species	Spectral Range (cm^{-1})		
	400 - 2000	2000 - 5000	5000 +
Diatomics	D	D/R	D
Metal oxides	D	D	-
NO_2, O_3	T	T/R	-
N_2O, CH_4 (T < 500 K)	A	A/R	-
N_2O (T > 500 K)	B/WF	B/WF	-
CO_2 (T < 500 K)	T	T	A
CO_2 (T > 500 K)	T	T	-
H_2O (T < 500 K)	A	A/R	A/WA
H_2O (T > 500 K)	L/WF	L/R	L/WF
HNO_3 (T < 300 K)	G	-	-

Notes:

D = DATE (Diatomic Thermal Emission) code (Reference 2-3)

R = Data same as ROSCOE-IR (Reference 2-1)

T = TATE (Triatomic Thermal Emission) code (Reference 2-3)

A = AFGL line-by-line data tape (Reference 2-5)

B = Boxcar (rectangular) band shape

WF = Retained old WOE fireball model (Reference 2-6)

WA = Retained old WOE ambient model (Reference 2-7)

L = Data obtained by Ludwig, et al (Reference 2-8)

G = Data obtained by Goldman, et al (Reference 2-4).

$$2\left(\alpha_L^i \cdot \mathrm{SOD} \cdot \mathrm{DEI}\right)^{1/2}$$

for each molecule for the temperatures 300 and 3000 K. In each case the curves labeled "1" represent the 300 K value, and the curves labeled "2" represent the 3000 K value. The Lorentz half-width α_L^i is determined according to

$$\alpha_L^i = \alpha_L^i(\mathrm{STP})\sqrt{273/T} \quad . \tag{2-2}$$

(The weak line parameter describes absorption for optically thin paths; the strong line parameter describes absorption for thick paths. In particular, the strong line parameter defines the square root region of the curve of growth for a statistical band.) Parameter values less than 10^{-7} are not shown in the figures; horizontal lines at 10^{-7} are artifacts of the plotting routine.

REFERENCES

2-1. Stephens, T.L., V.R. Stull, A.L. Klein, and J.D. Losse, *The [illegible] Manual, Volume 2S—Molecular Band Models for Thermal and Optically Pumped Emissions*, Unpublished.

2-2. Stanton, M.J., et al, *Nuclear-Induced Optical Phenomenology Program*, Unpublished.

2-3. Stephens, T.L., and J.G. DeVore, *Band Model Parameters for Thermal Emission*, Unpublished.

2-4. Goldman, A., T.G. Kyle, and F.S. Bonomo, *Statistical Band Model Parameters and Integrated Intensities for the 6.3 μ, 7.5 μ, and 11.3 μ Bands of HNO_3 Vapor*, AFCRL-70-0091, Air Force Cambridge Research Laboratories, January 1970.

2-5. McClatchey, R.A., et al, *AFCRL Atmospheric Line Parameters Compilation*, AFCRL-TR-73-0096, Air Force Cambridge Research Laboratories, January 1973; updated data tape supplied July 1977.

2-6. Ewing, L.E., *Modeling Detail in the Weapon Optical Effects Code*, Unpublished.

2-7. Stephens, T.L., *Atmospheric Transmission in the [illegible] Range*, 68TMP-79, General Electric—TEMPO, July 1968, and Supplement.

2-8. Ferriso, C.C., C.B. Ludwig, and A.L. Thomson, "Empirically Determined Infrared Absorption Coefficients of H_2O from 300 to 3000°K," *J. of Quantitative Spectroscopy and Radiative Transfer*, vol 6, pp 241-273, 1966; and Ludwig, C.B., "Measurements of the Curve-of-Growth of Hot Water Vapor," *Applied Optics*, vol 10, no 5, 1971.

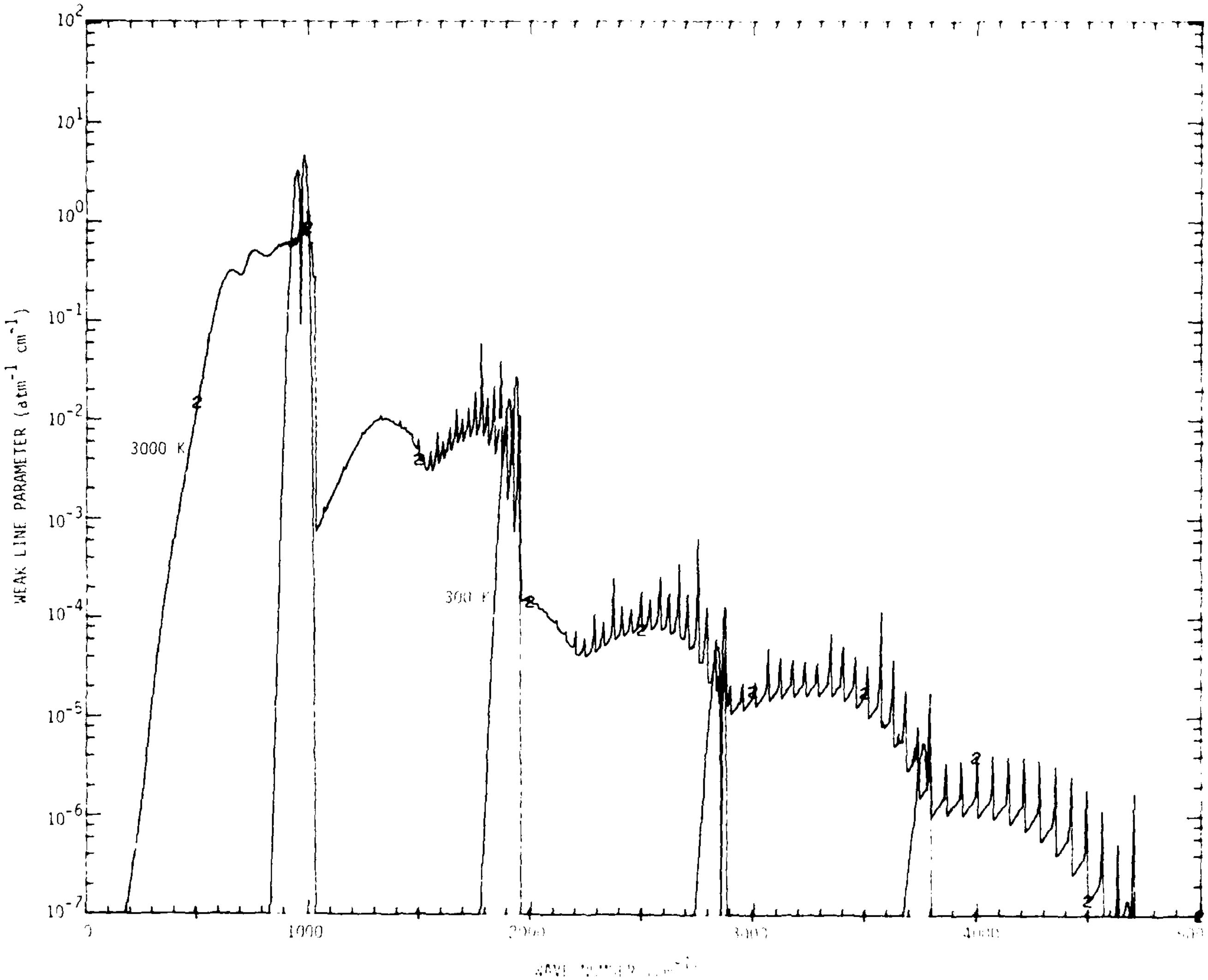

Figure 2-1. Weak line parameters for AℓO.

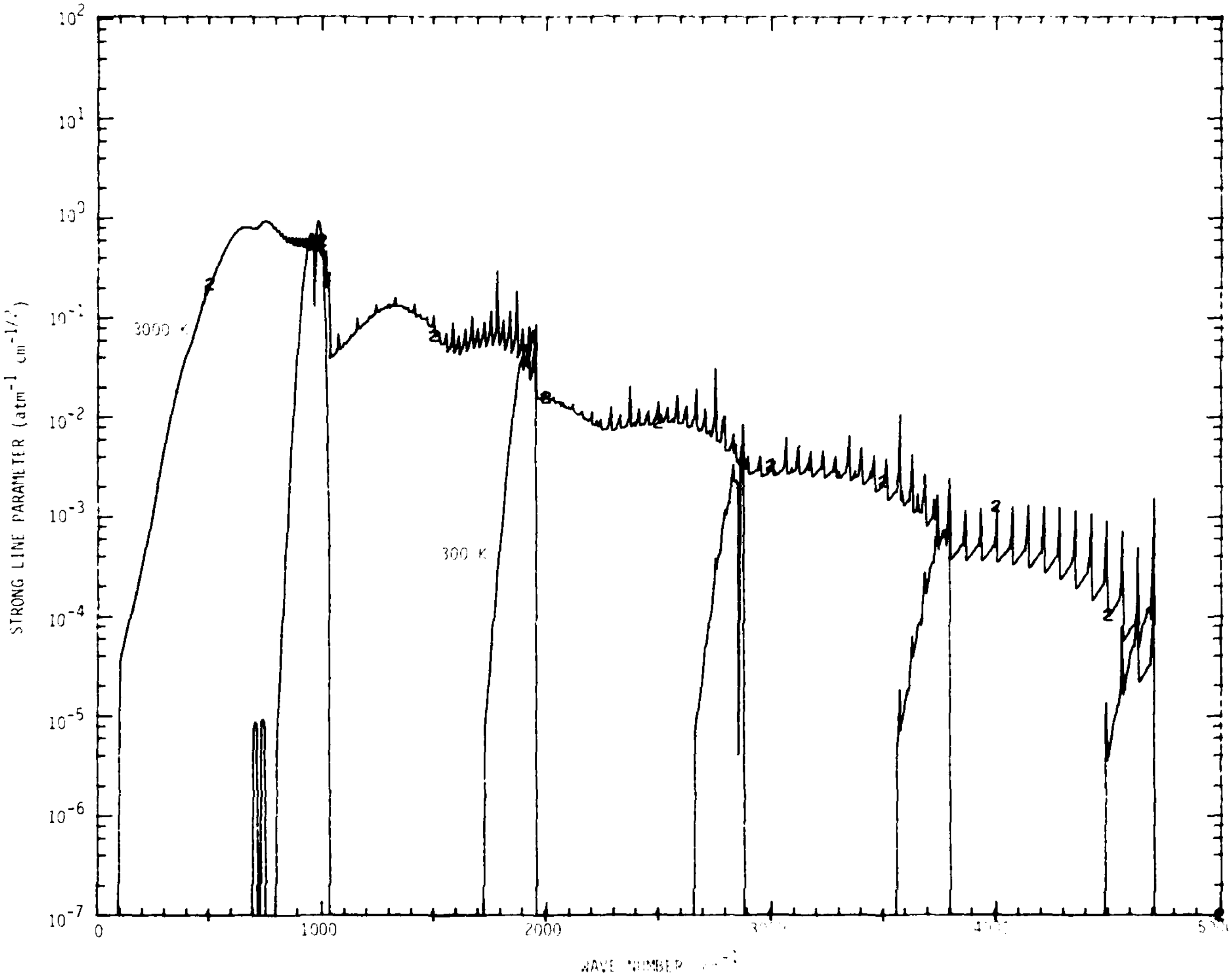

Figure 2-2. Strong line parameters for AlO.

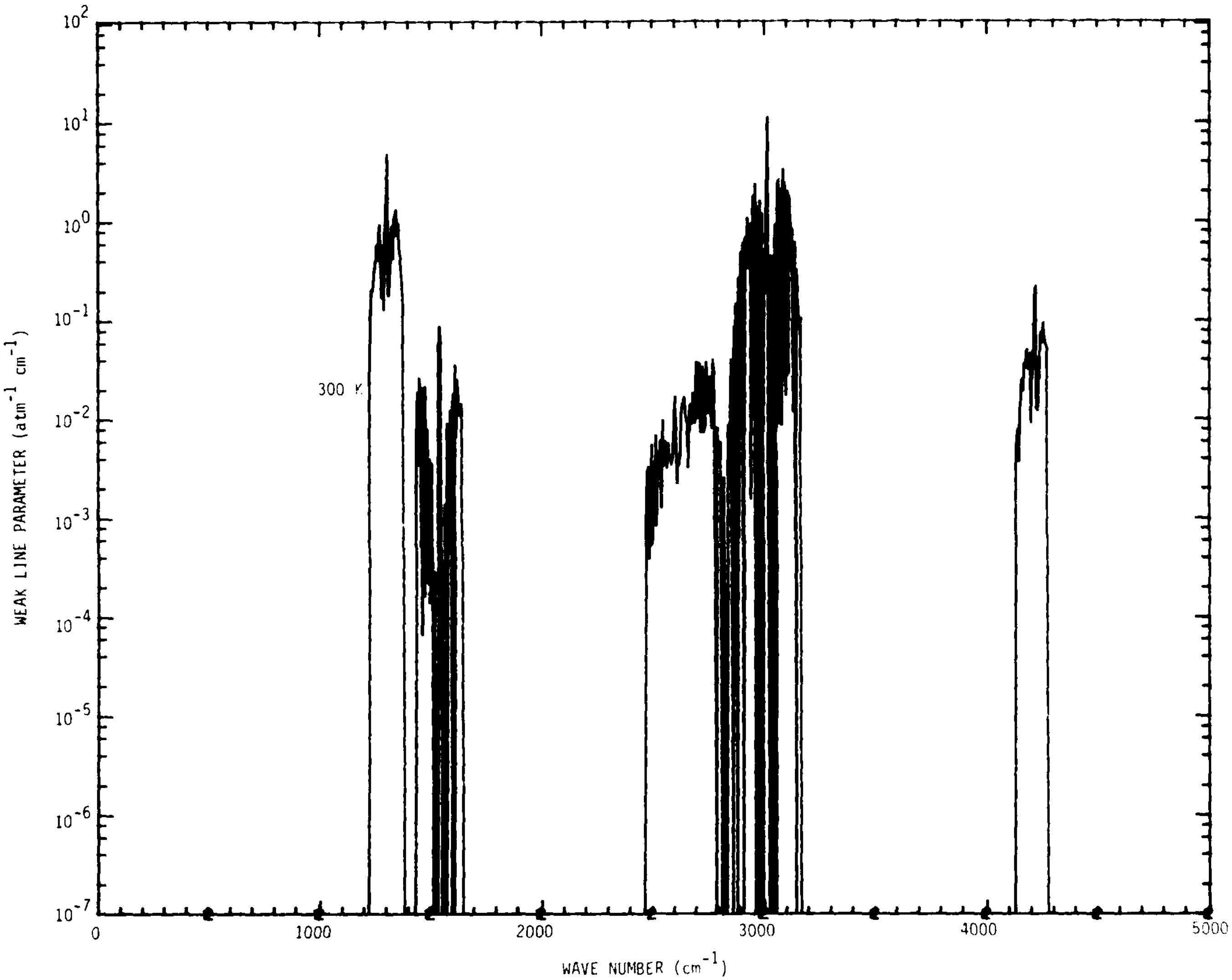

Figure 2-3. Weak line parameters for CH_4.

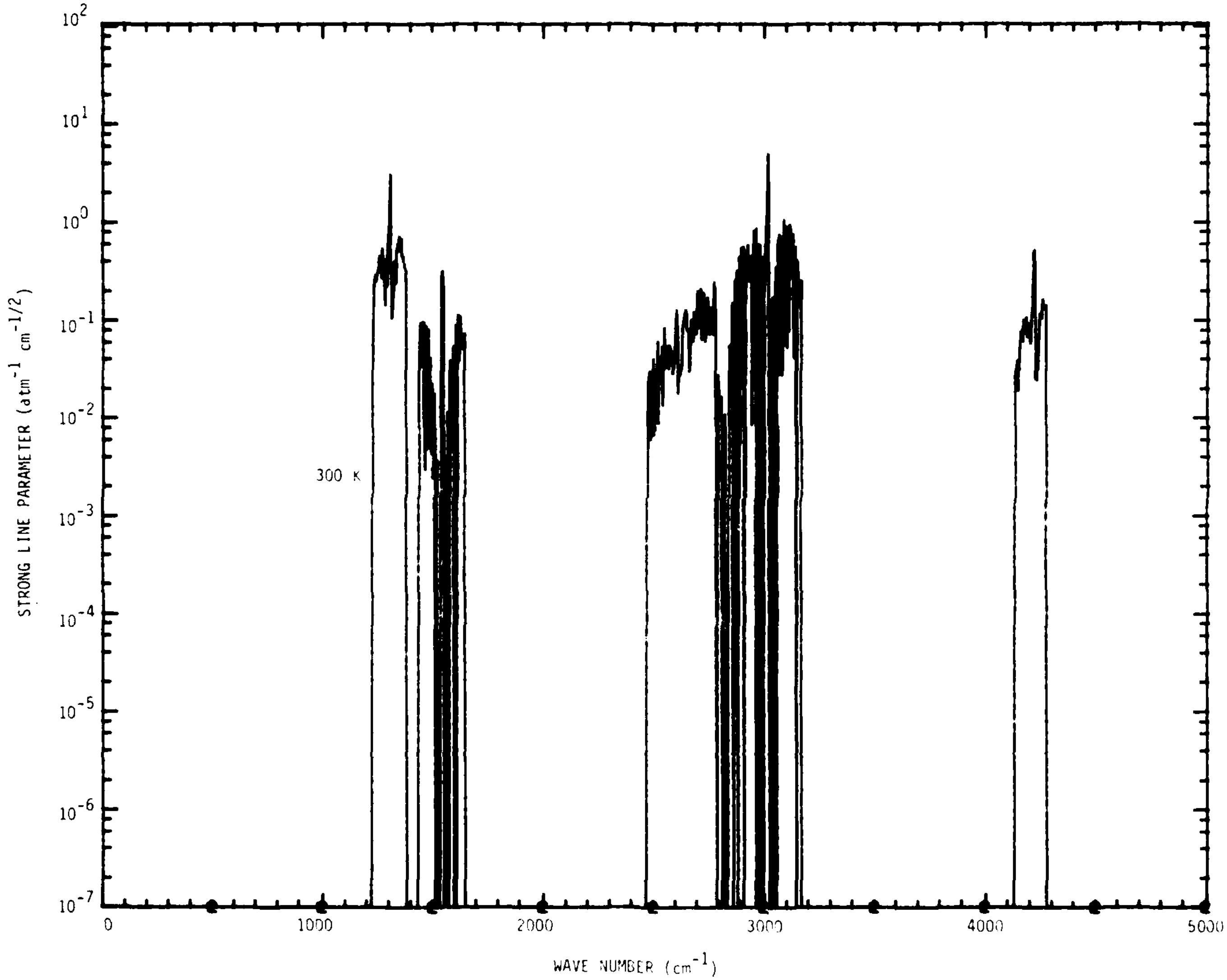

Figure 2-4. Strong line parameters for CH_4.

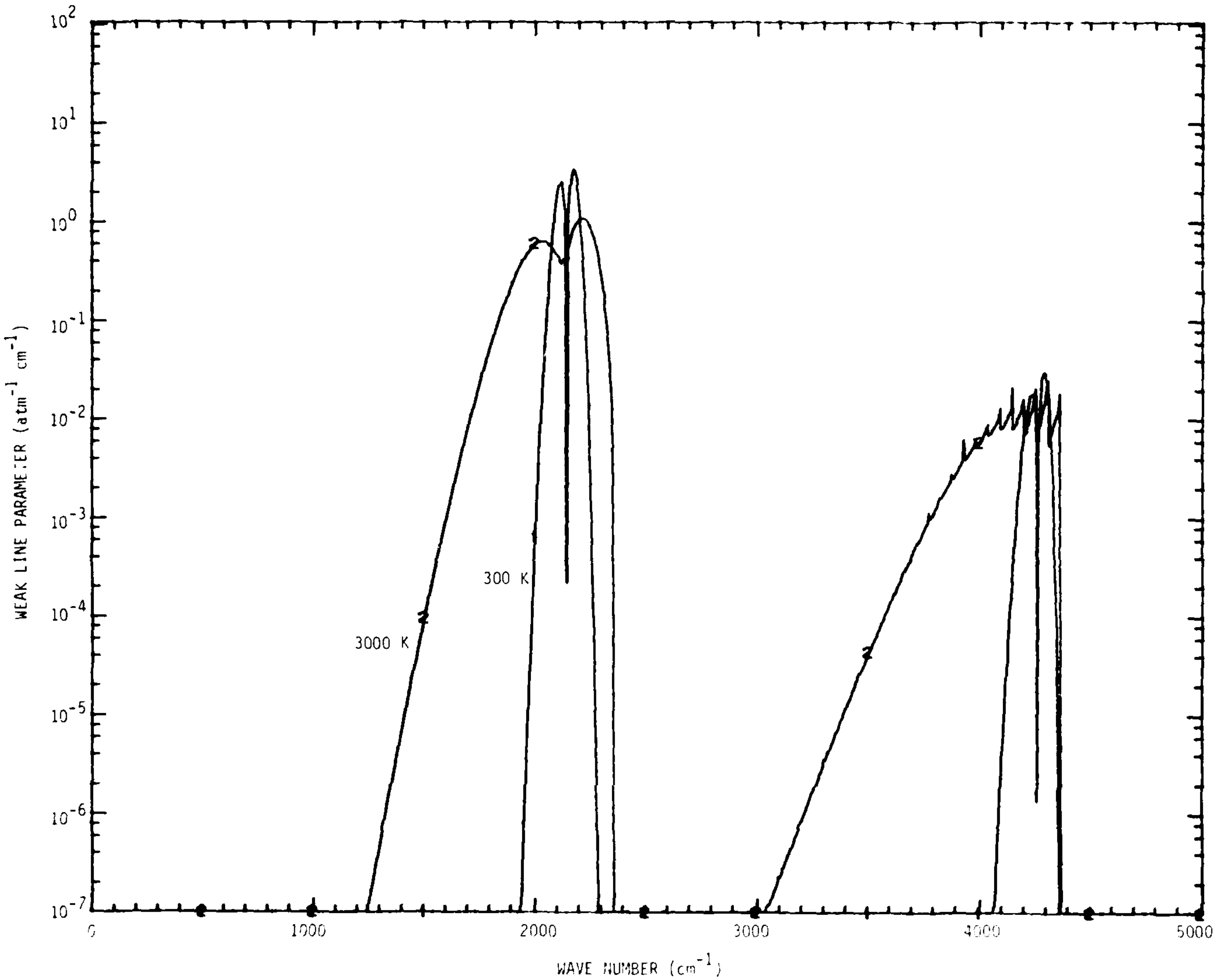

Figure 2-5. Weak line parameters for CO.

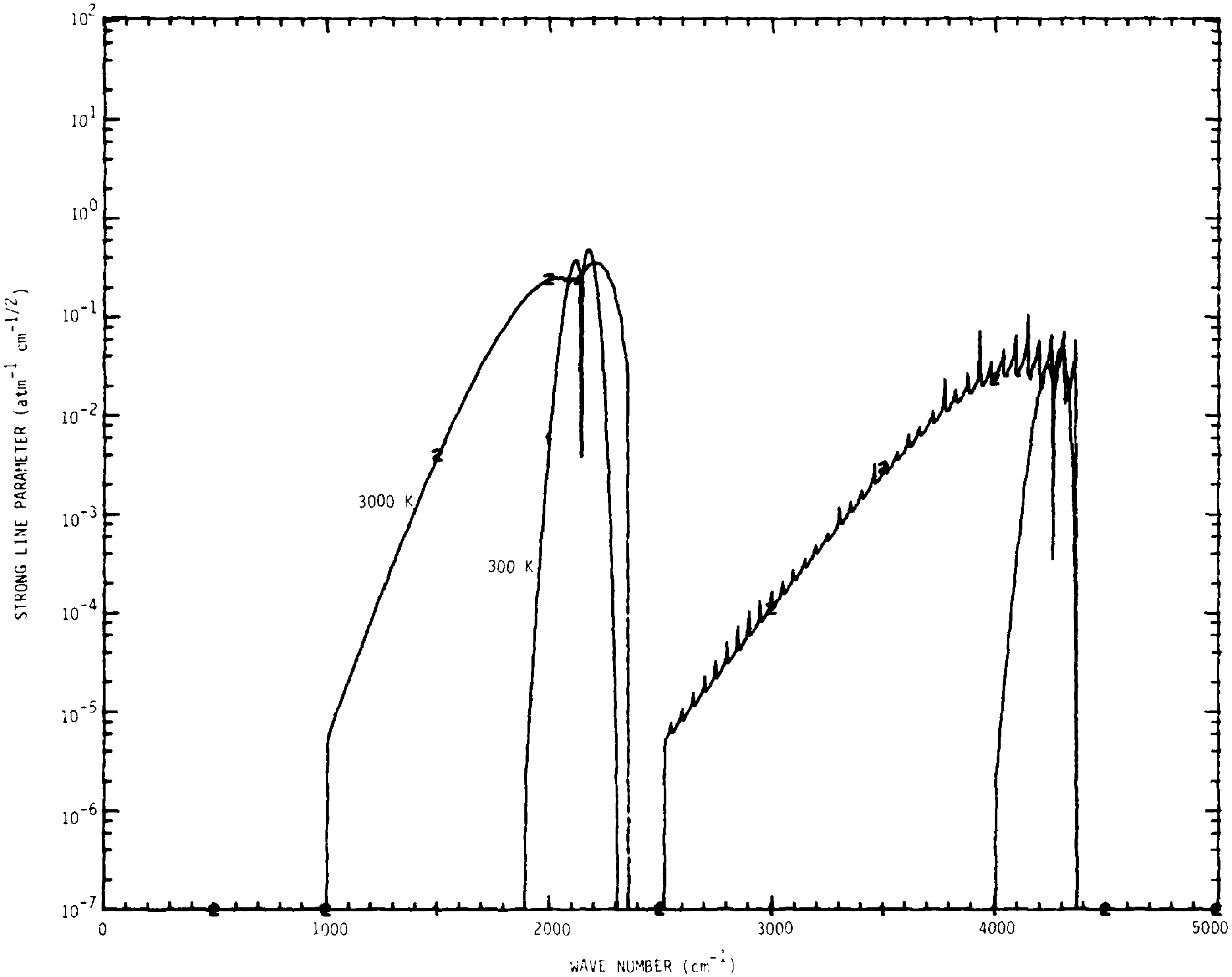

Figure 2-6. Strong line parameters for CO.

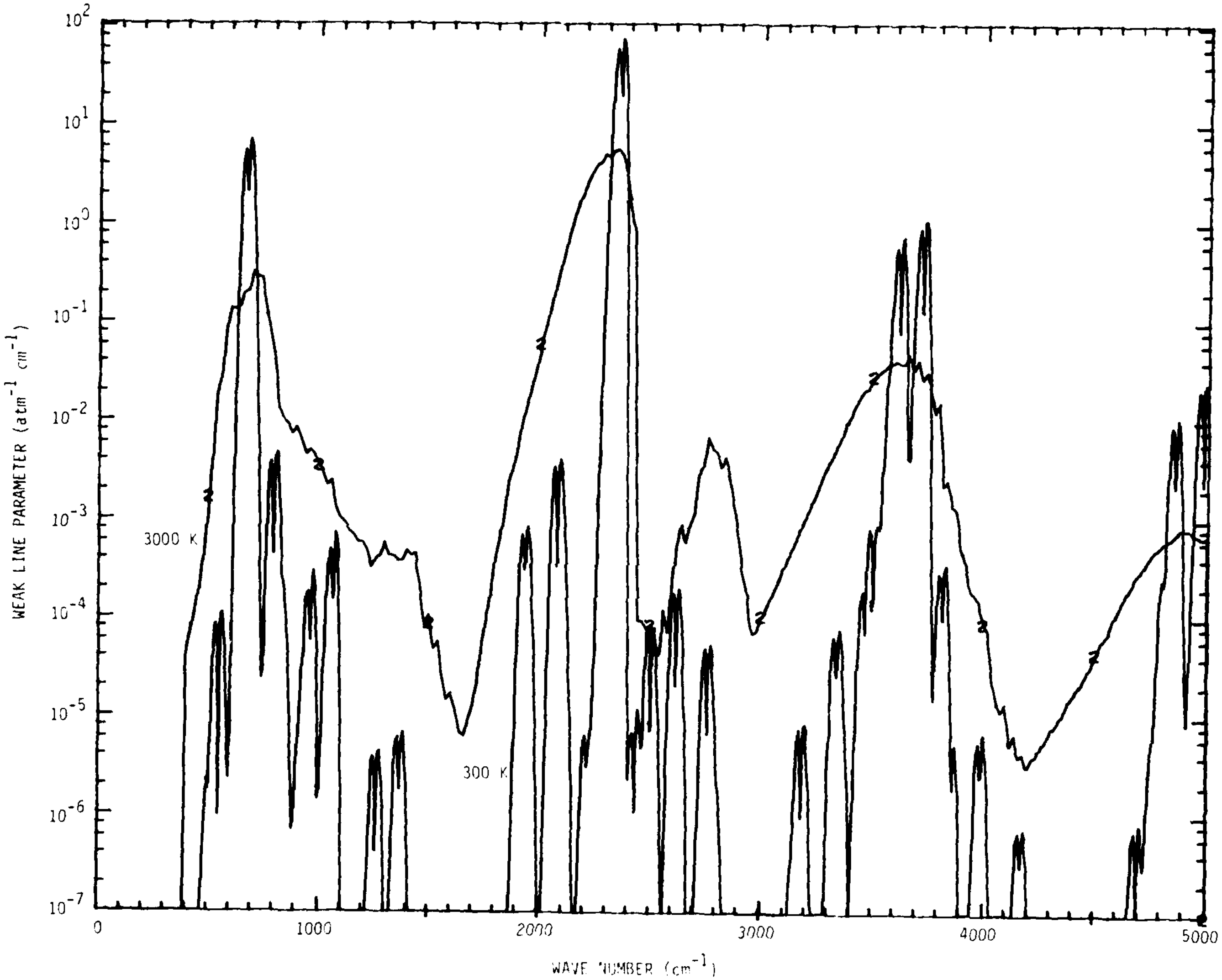

Figure 2-7. Weak line parameters for CO_2.

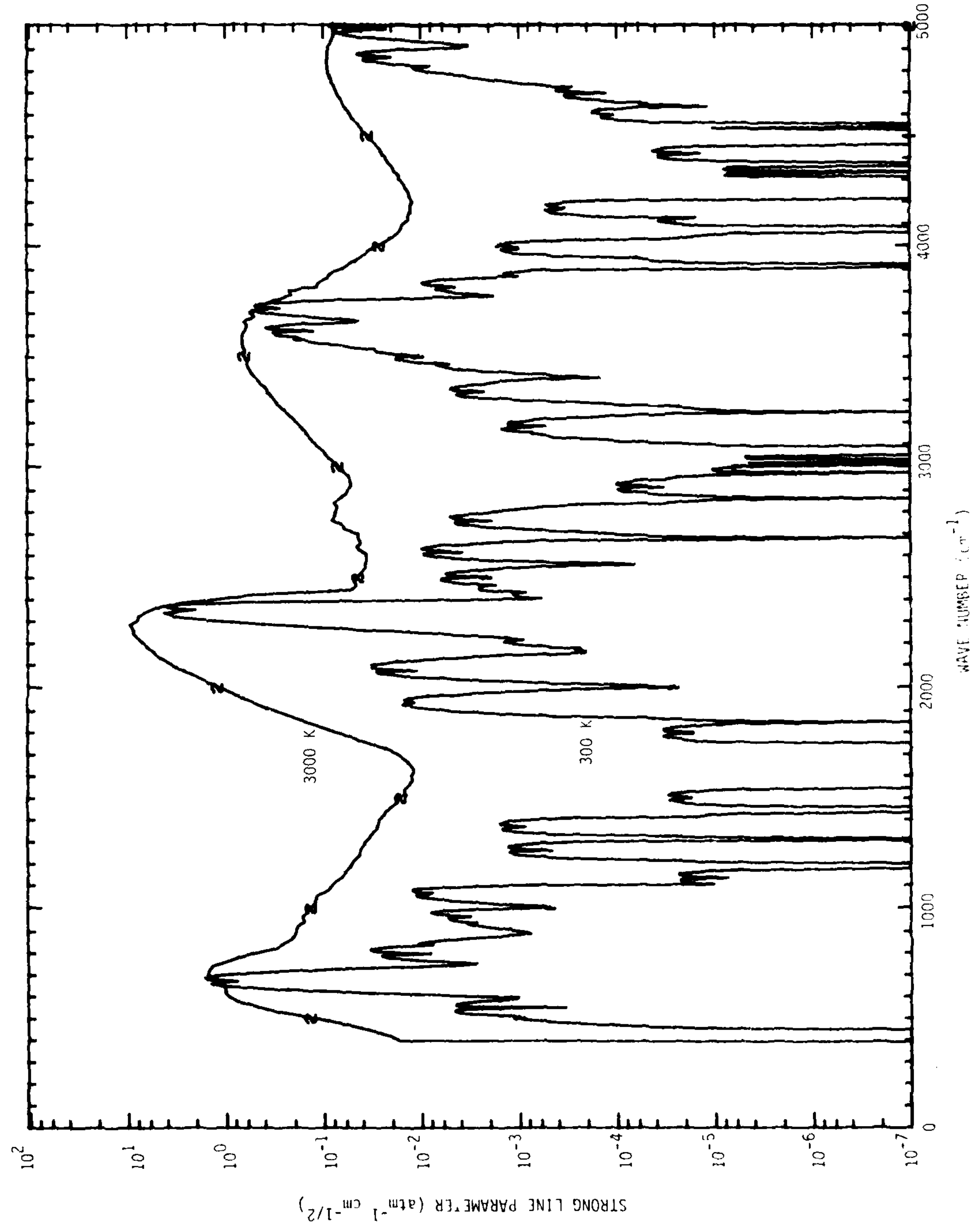

Figure 2-8. Strong line parameters for CO_2.

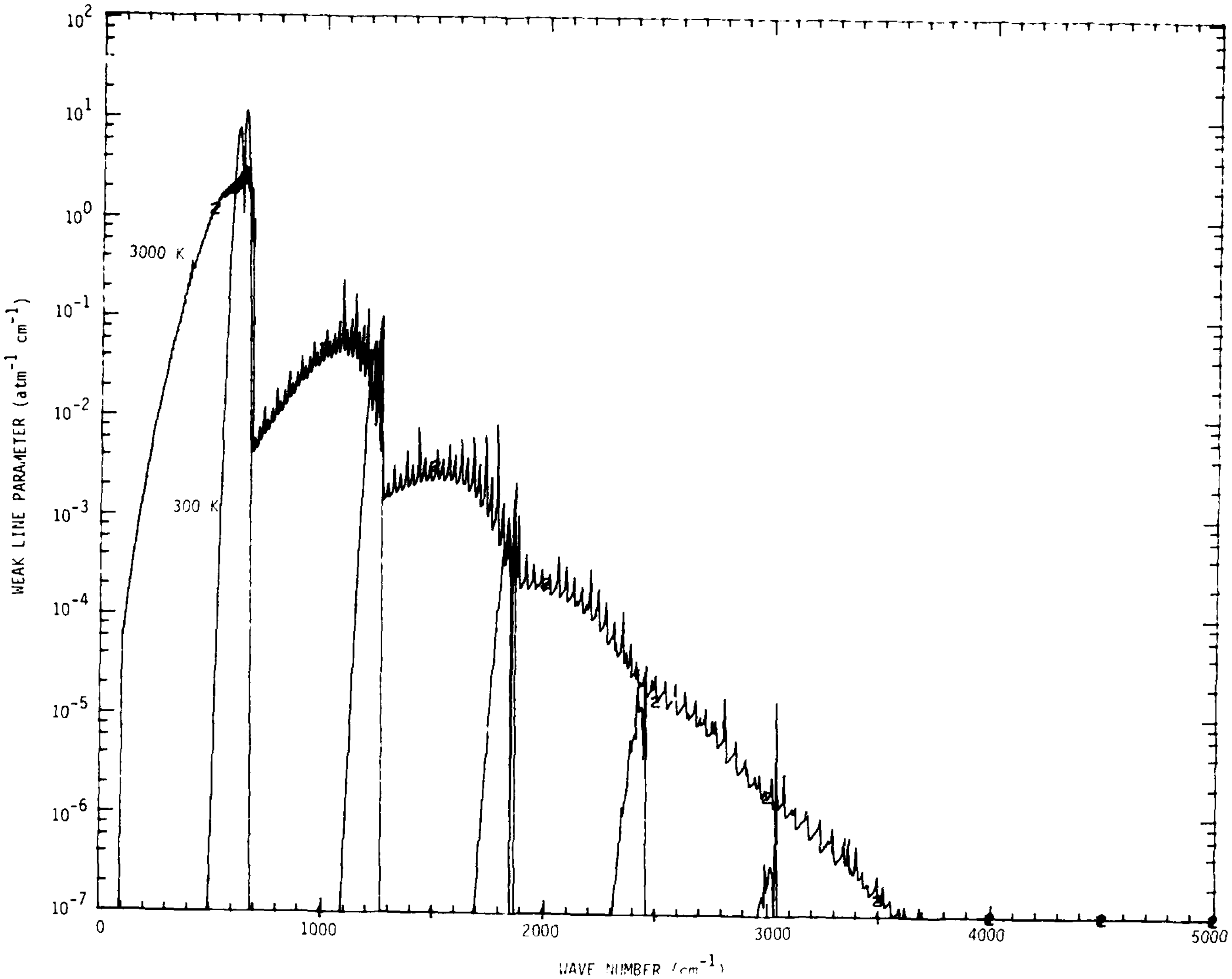

Figure 2-9. Weak line parameters for CuO.

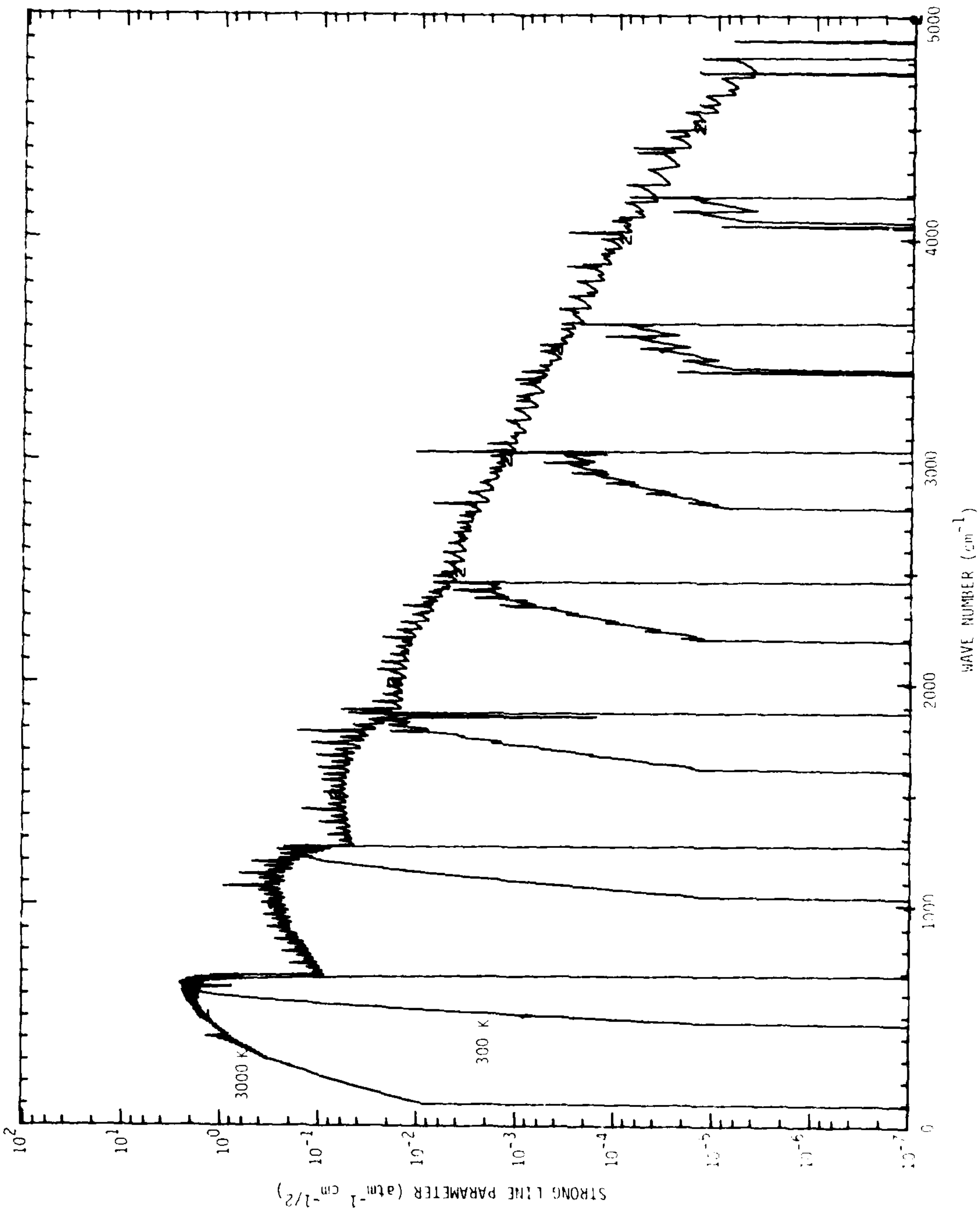

Figure 2-10. Strong line parameters for CuO.

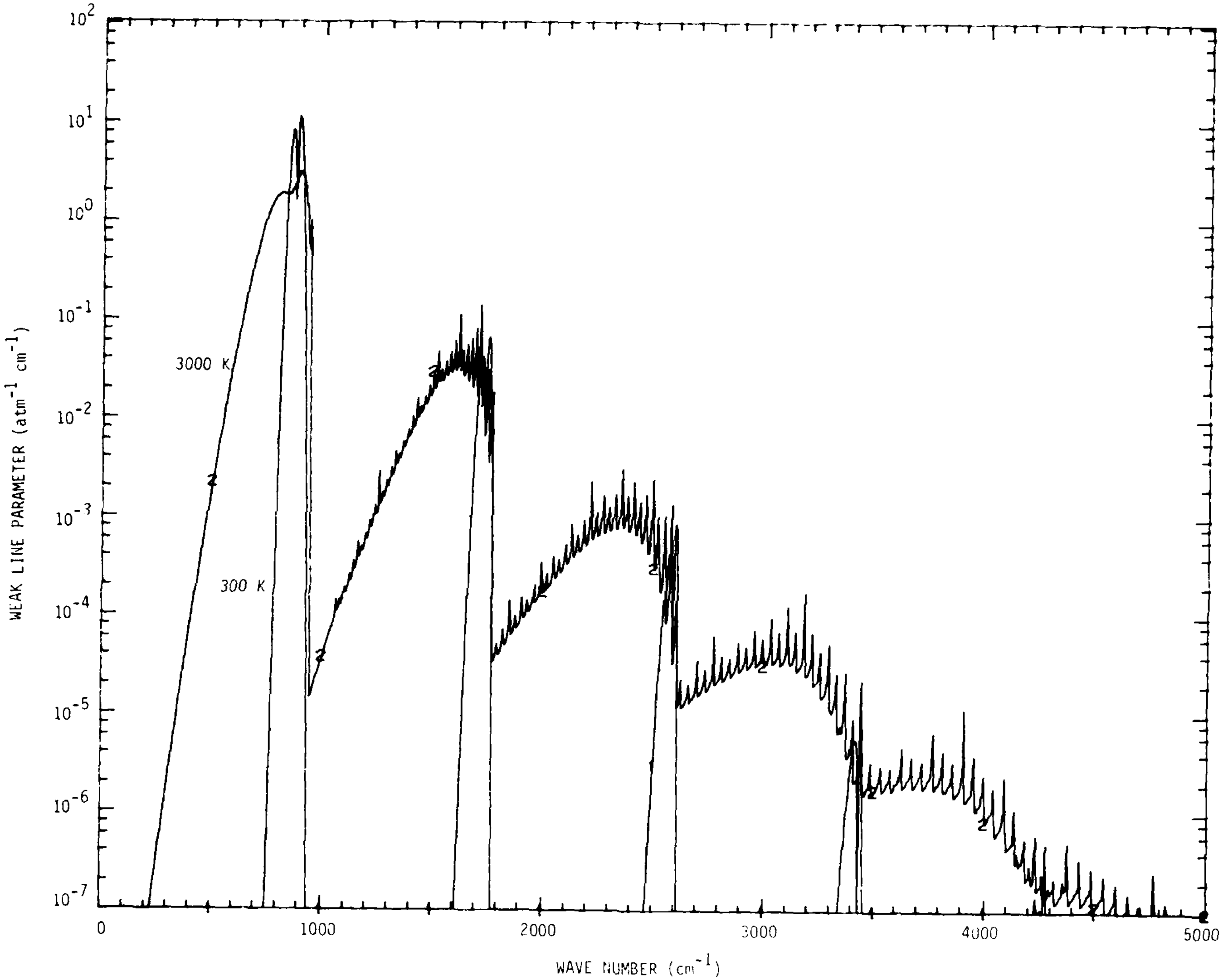

Figure 2-11. Weak line parameters for FeO.

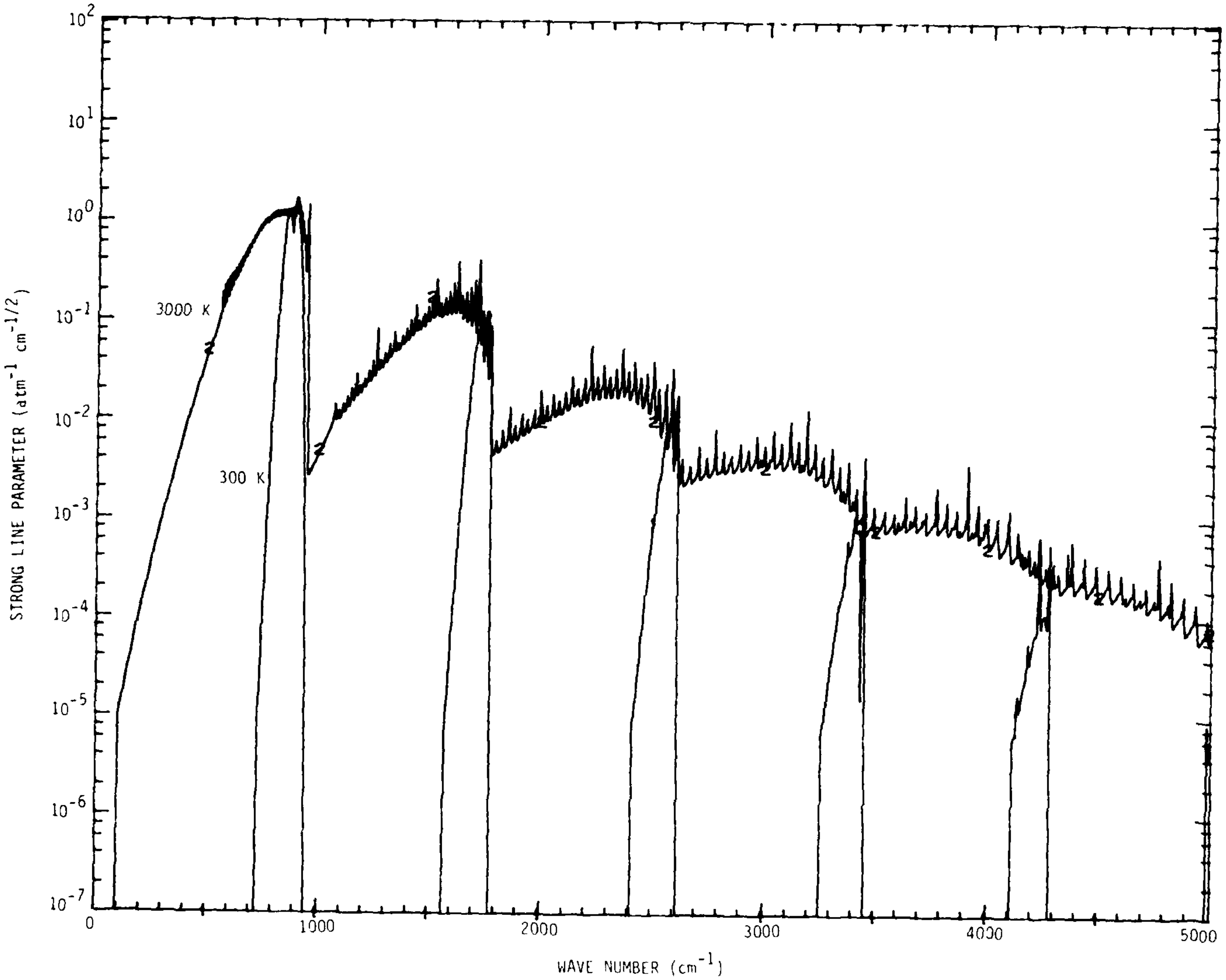

Figure 2-12. Strong line parameters for FeO.

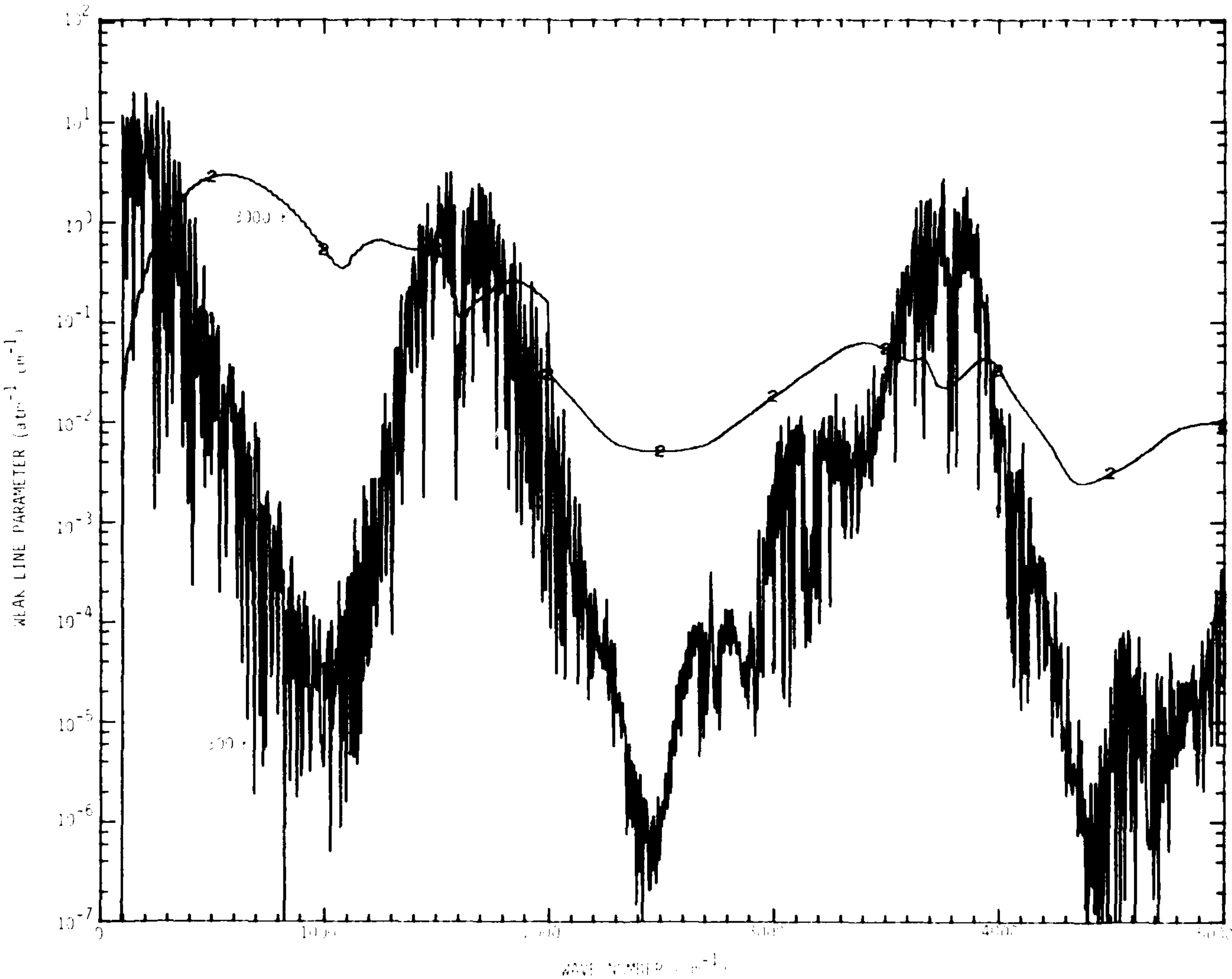

Figure 2-13. Weak line parameters for H_2O.

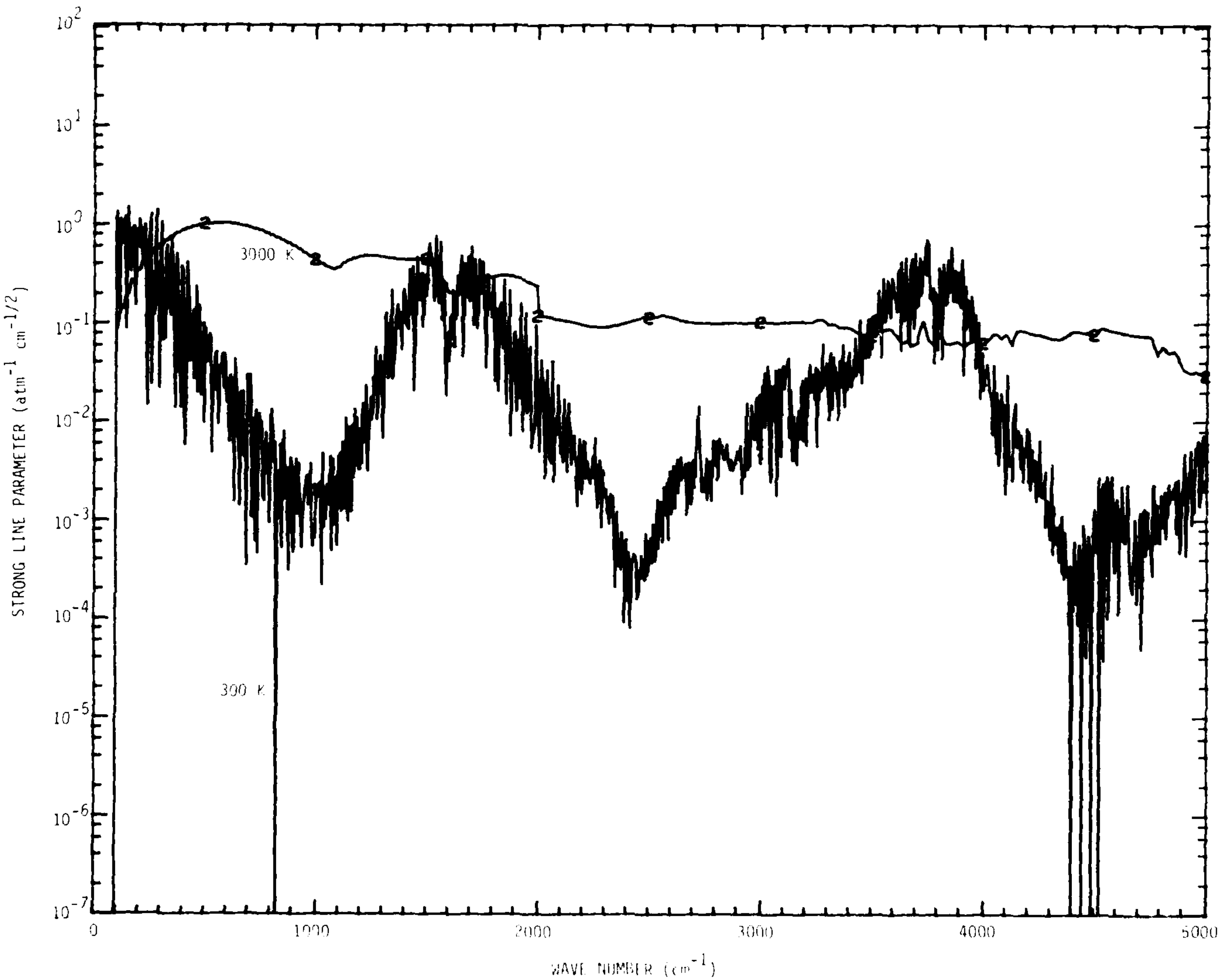

Figure 2-14. Strong line parameters for H_2O.

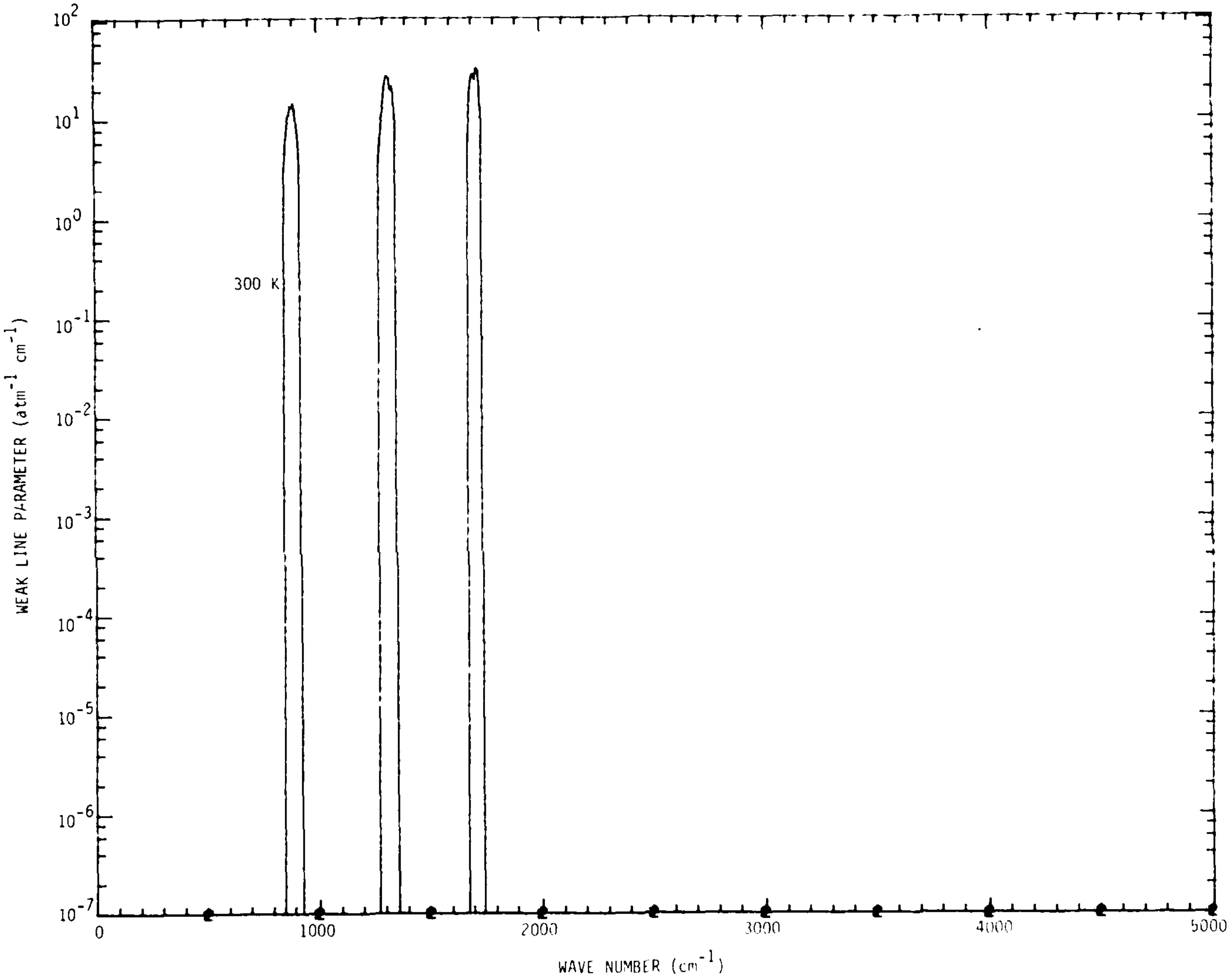

Figure 2-15. Weak line parameters for HNO_3.

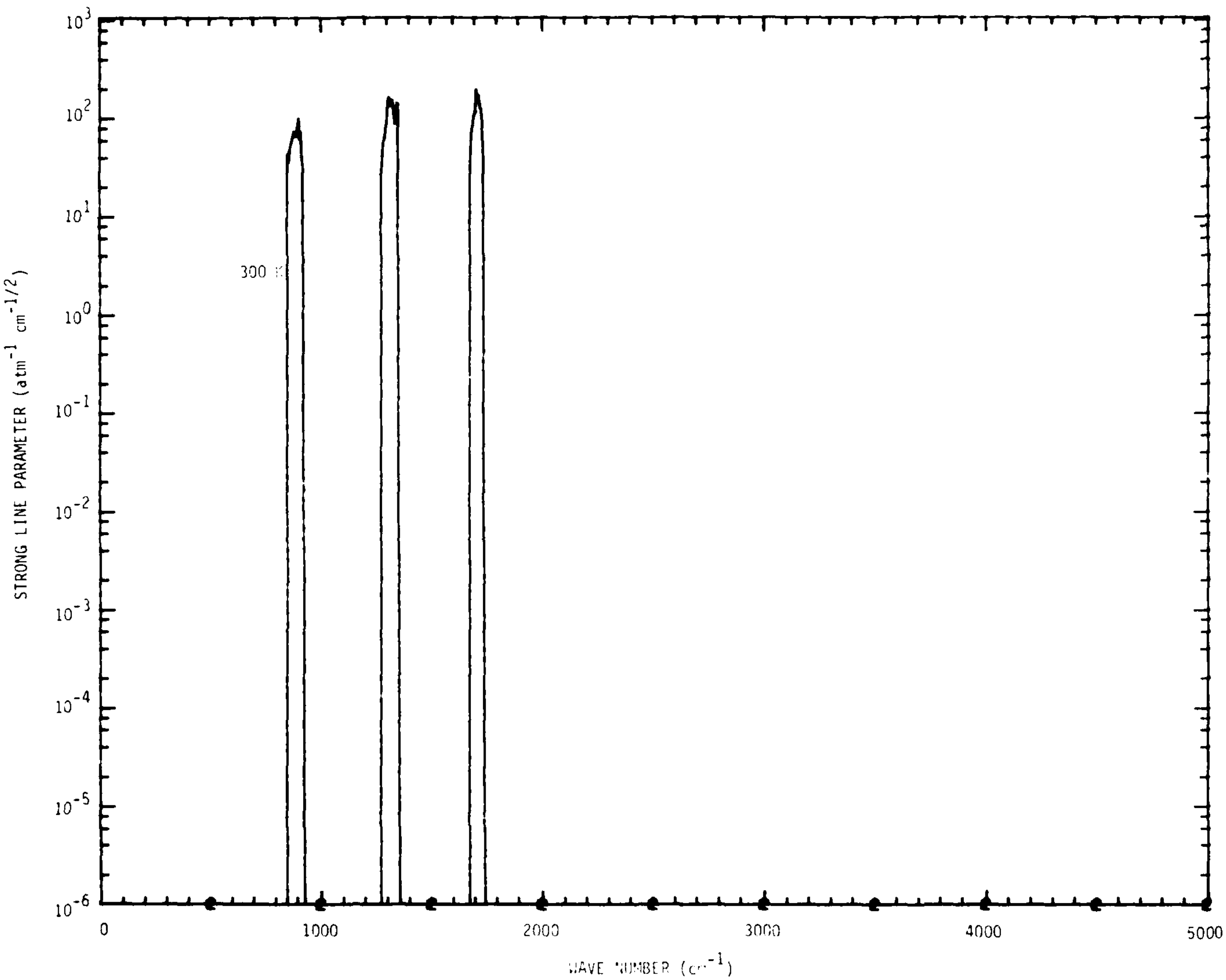

Figure 2-16. Strong line parameters for HNO_3.

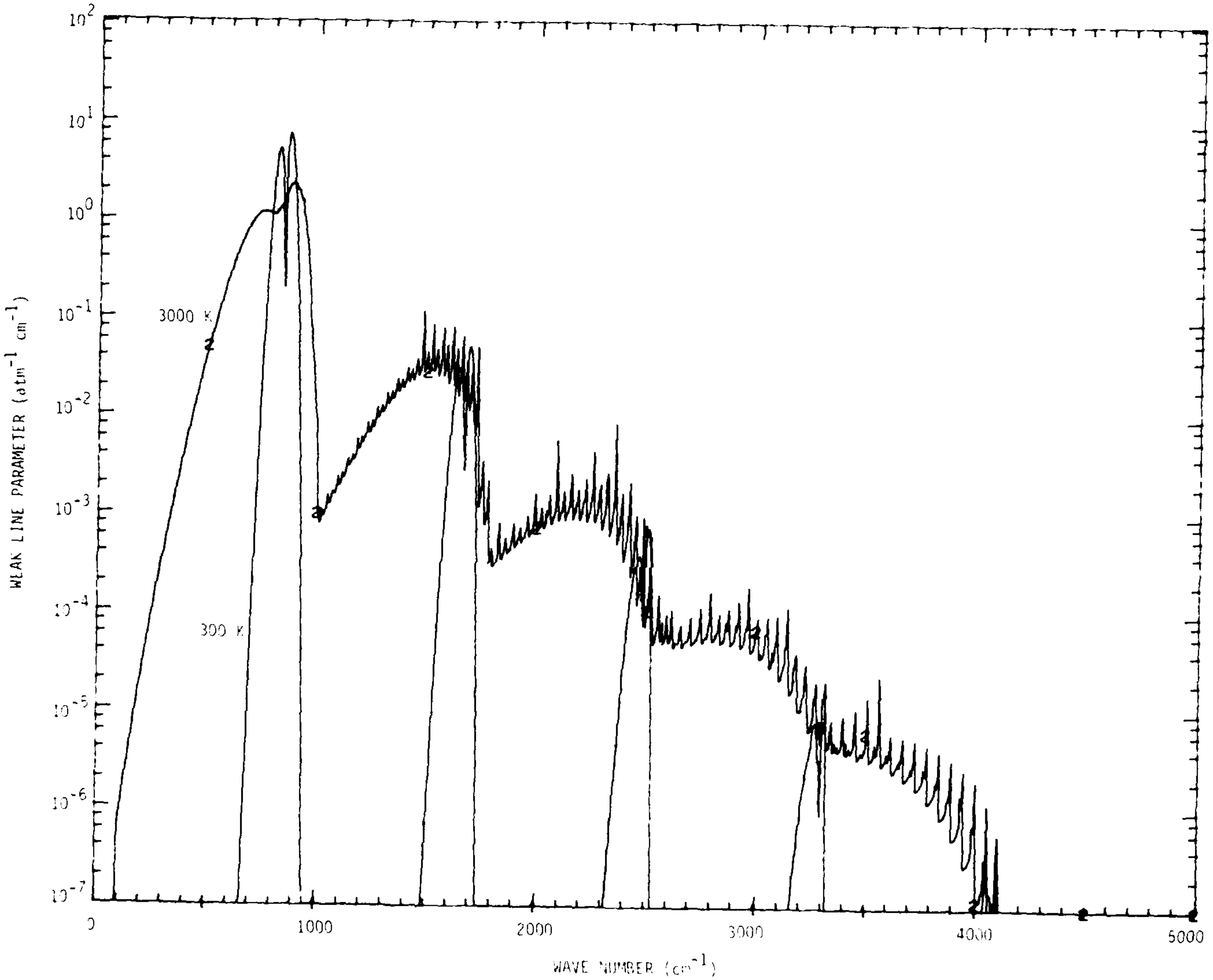

Figure 2-17. Weak line parameters for LiO.

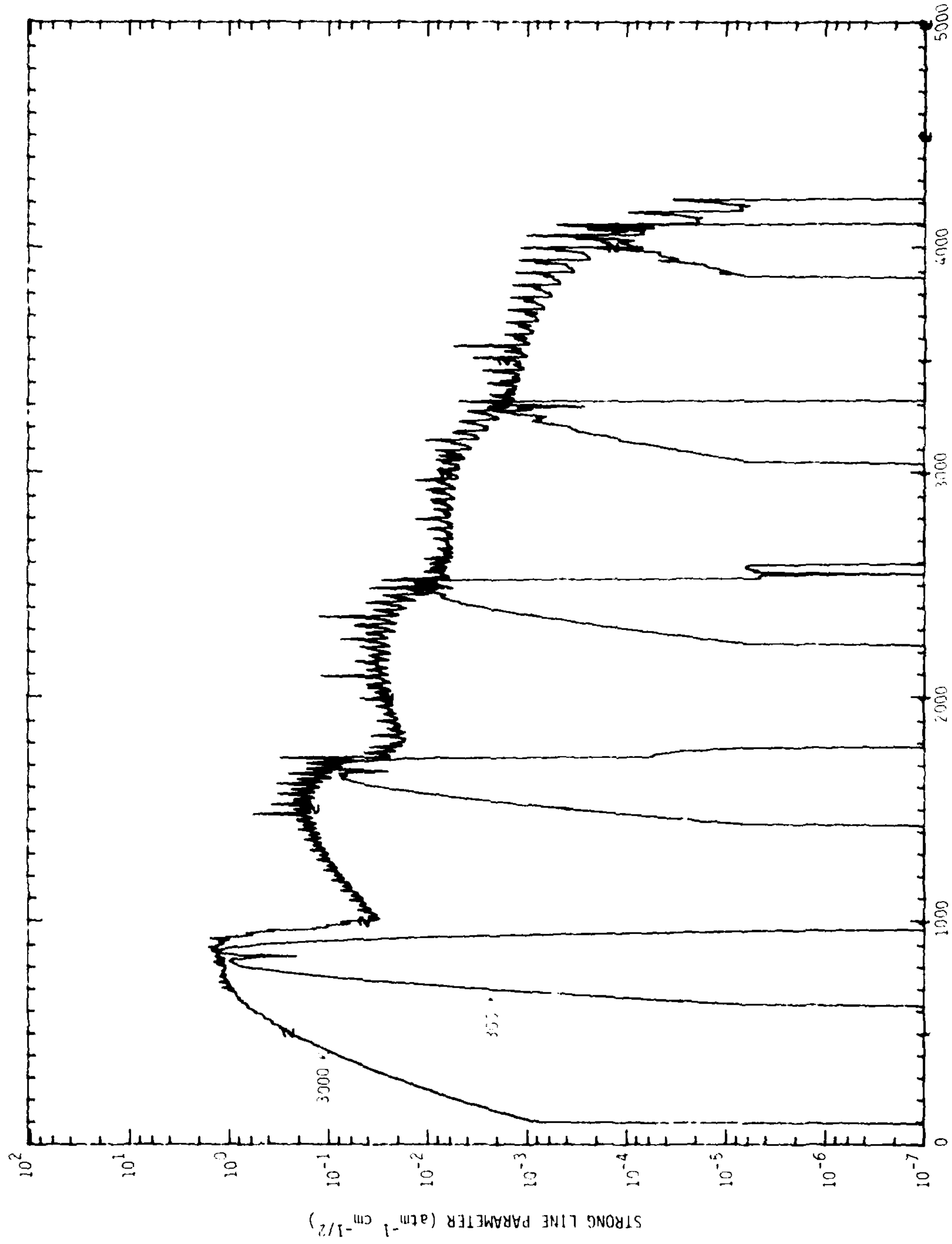

Figure 2-18. Strong line parameters for LiO.

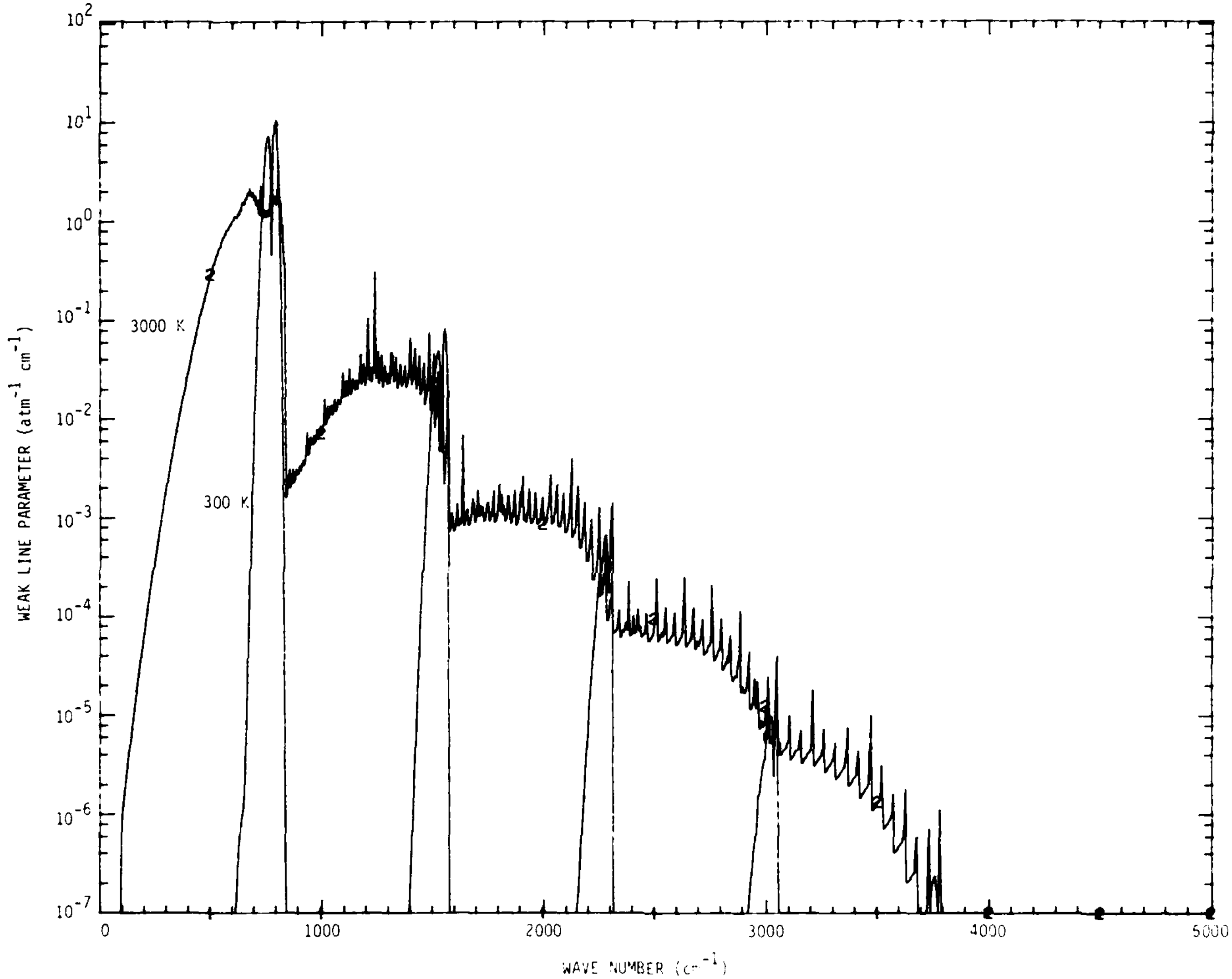

Figure 2-19. Weak line parameters for MgO.

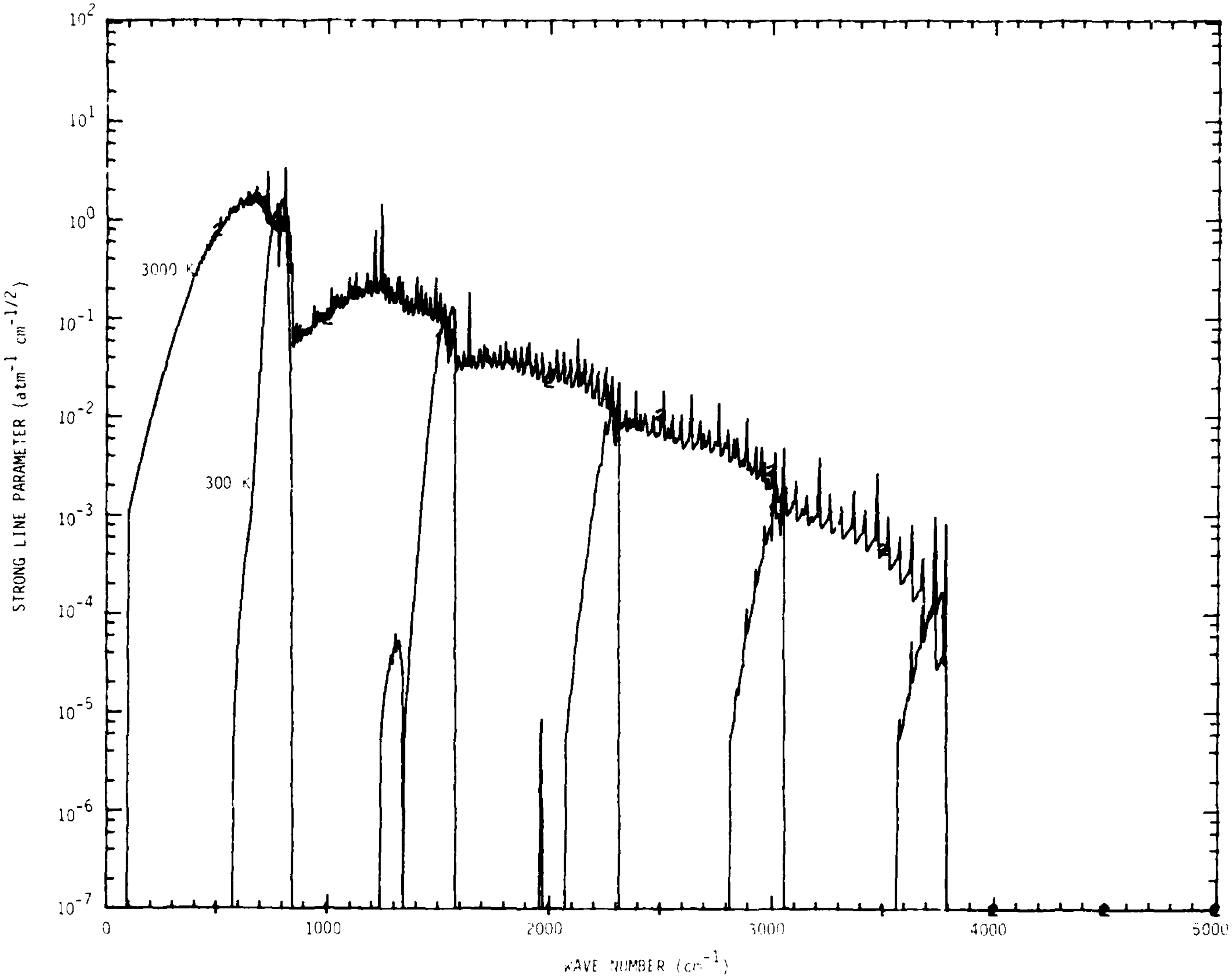

Figure 2-20. Strong line parameters for MgO.

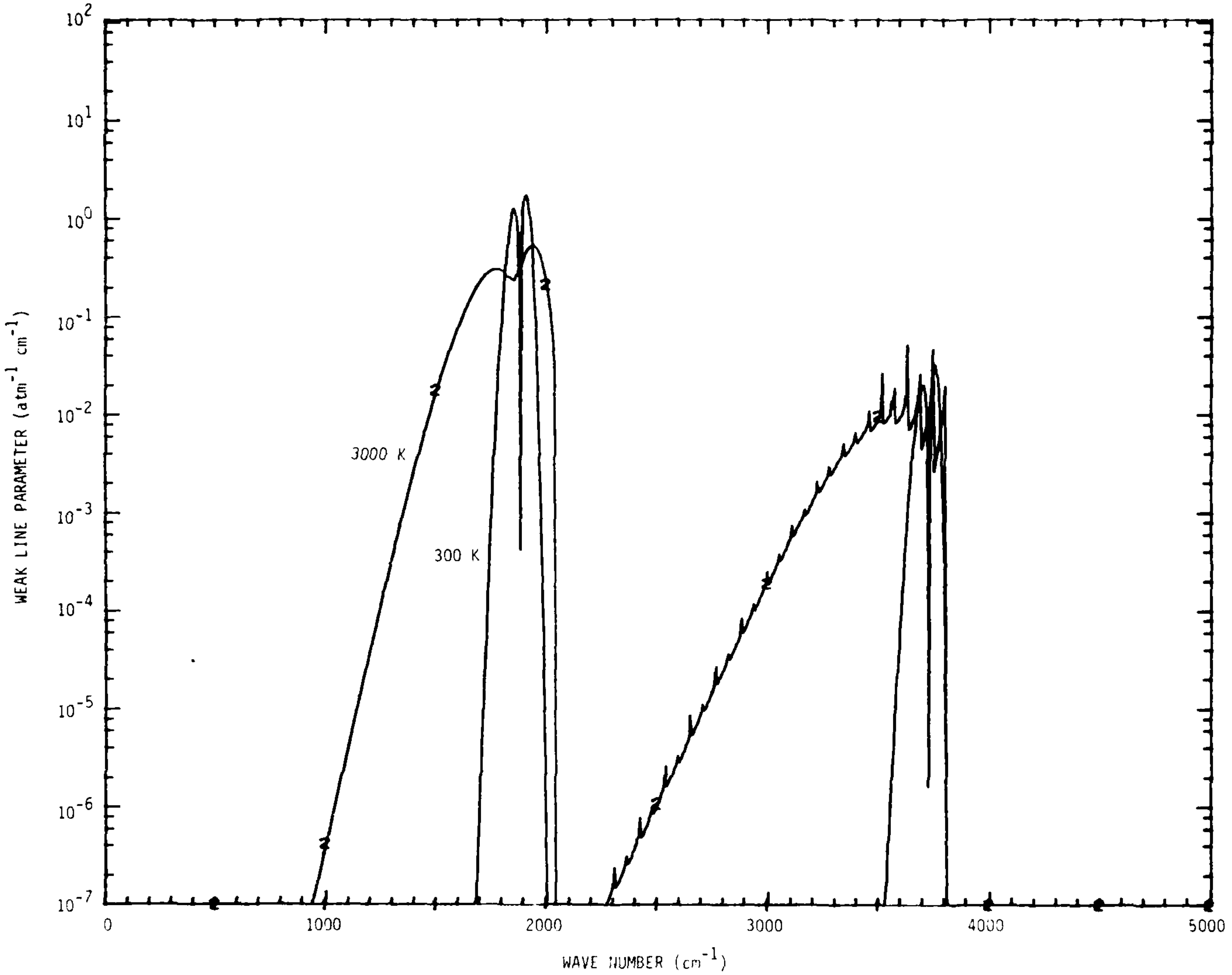

Figure 2-21. Weak line parameters for NO.

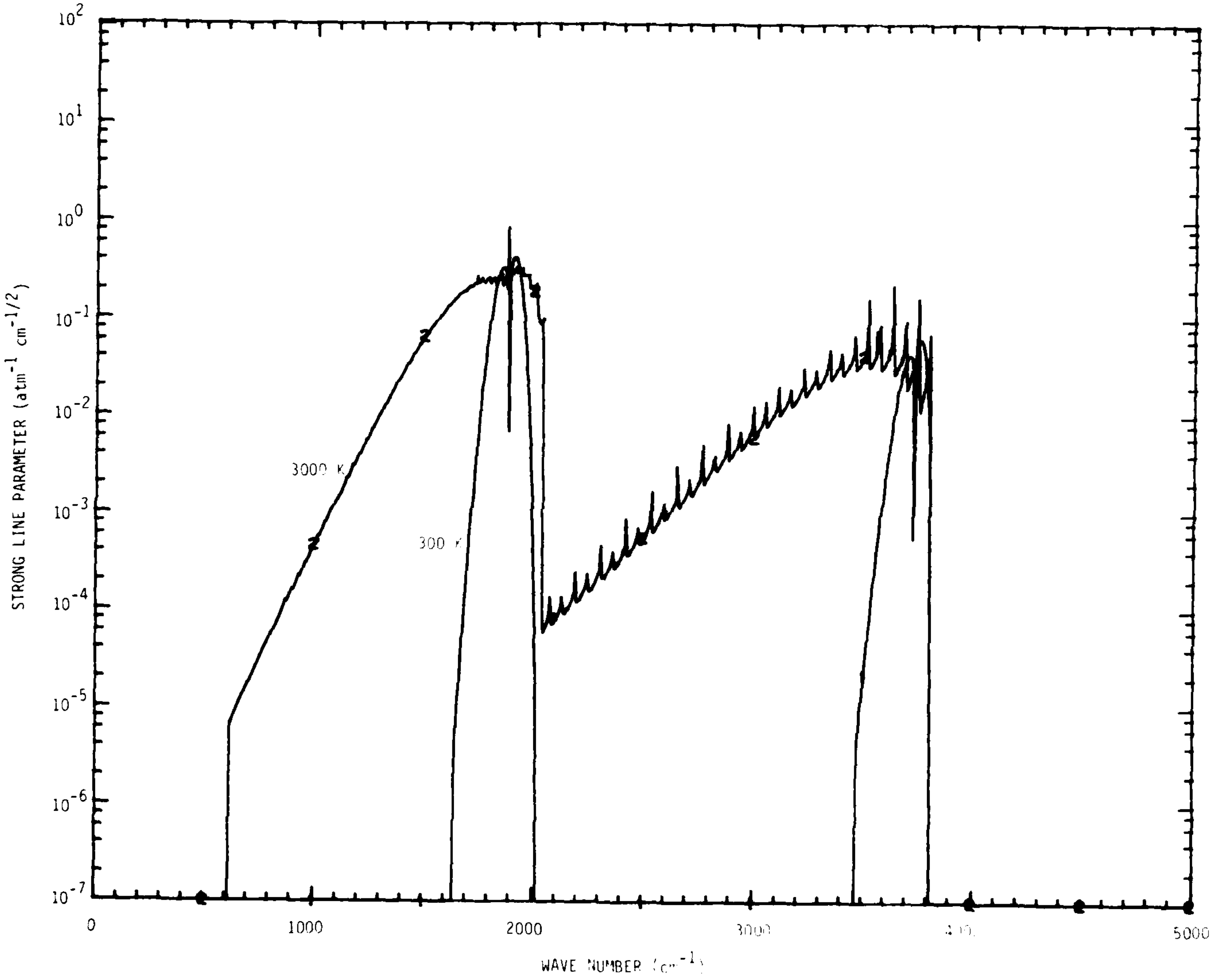

Figure 2-22. Strong line parameters for NO.

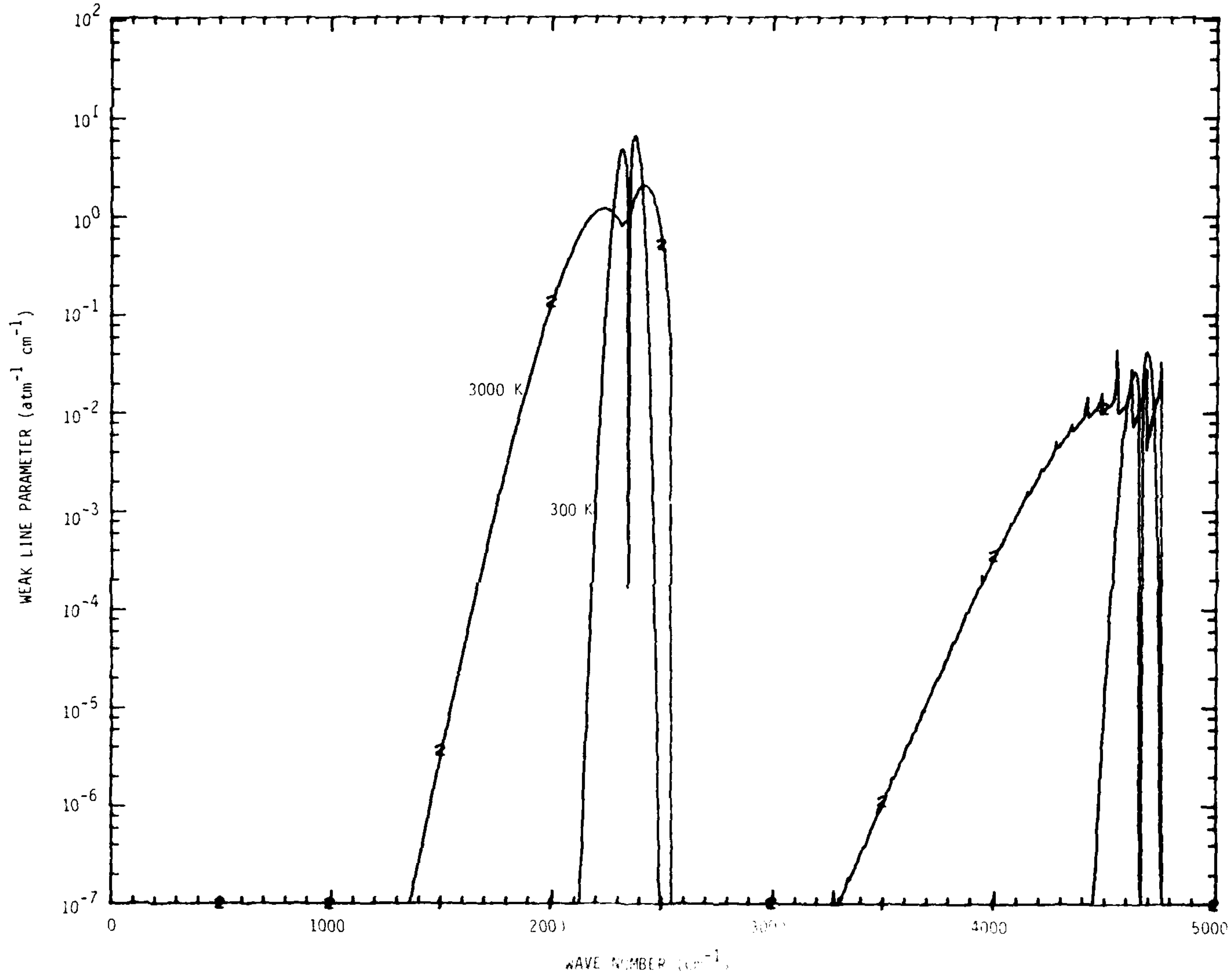

Figure 2-23. Weak line parameters for NO^+.

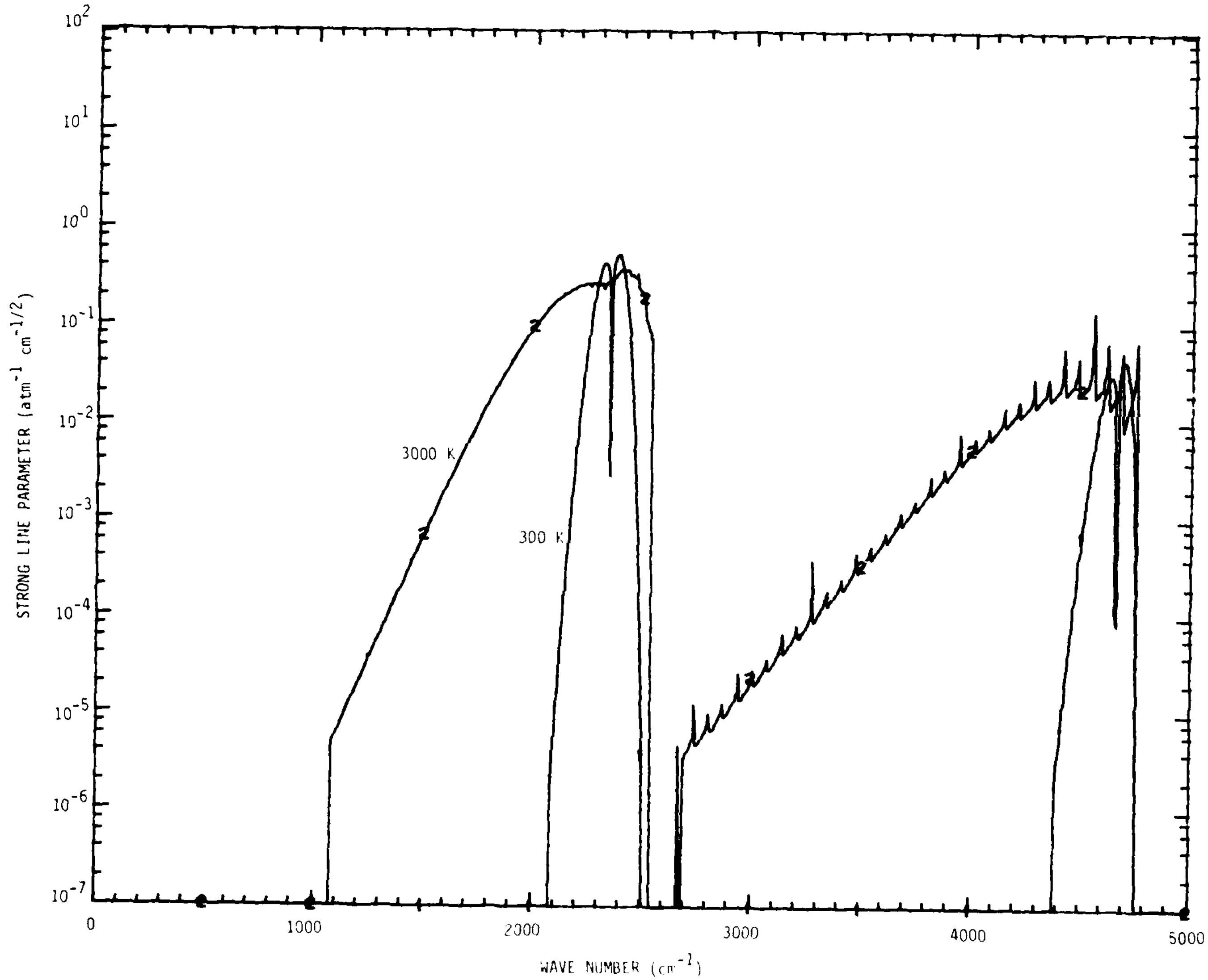

Figure 2-24. Strong line parameters for NO^+.

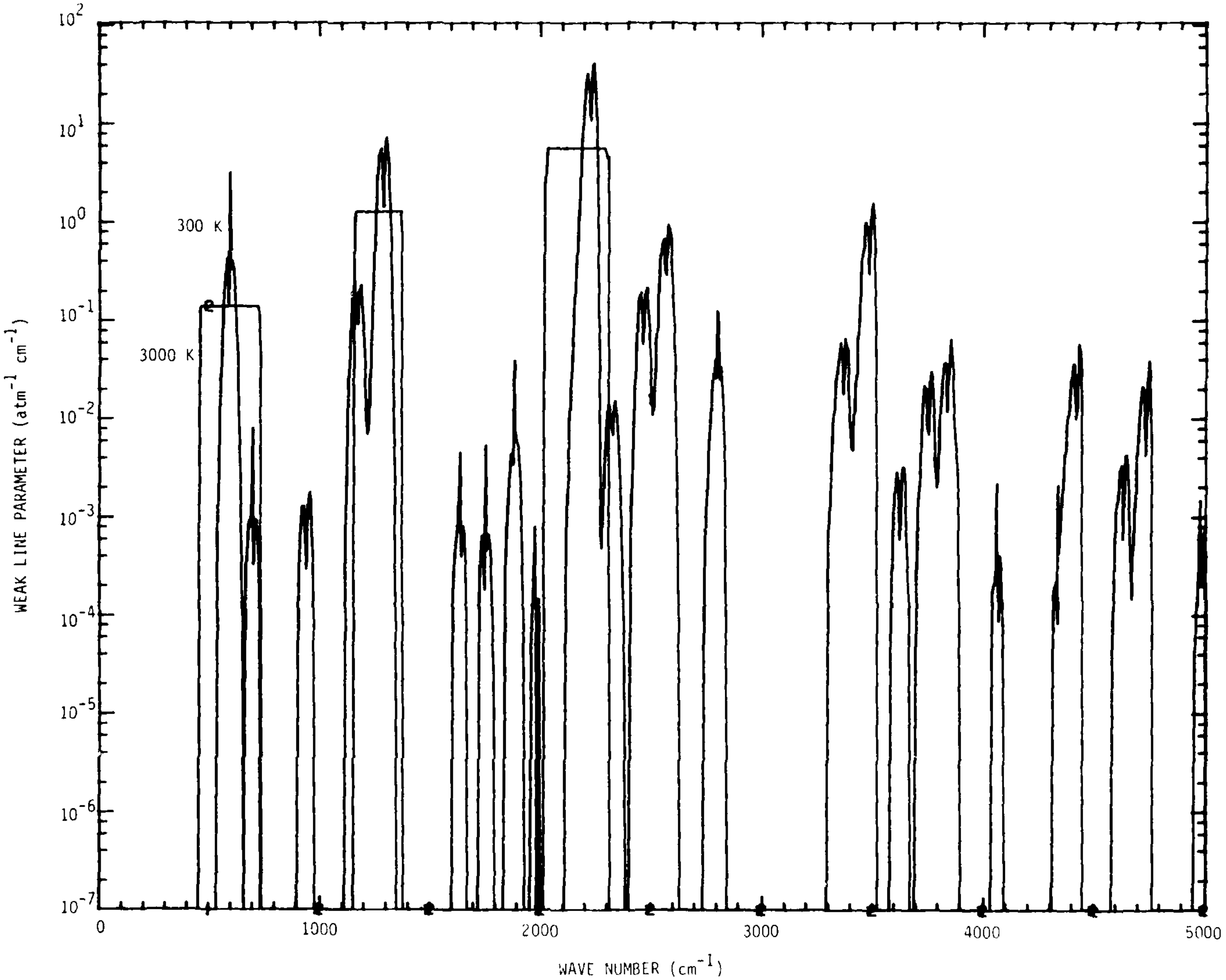

Figure 2-25. Weak line parameters for N_2O.

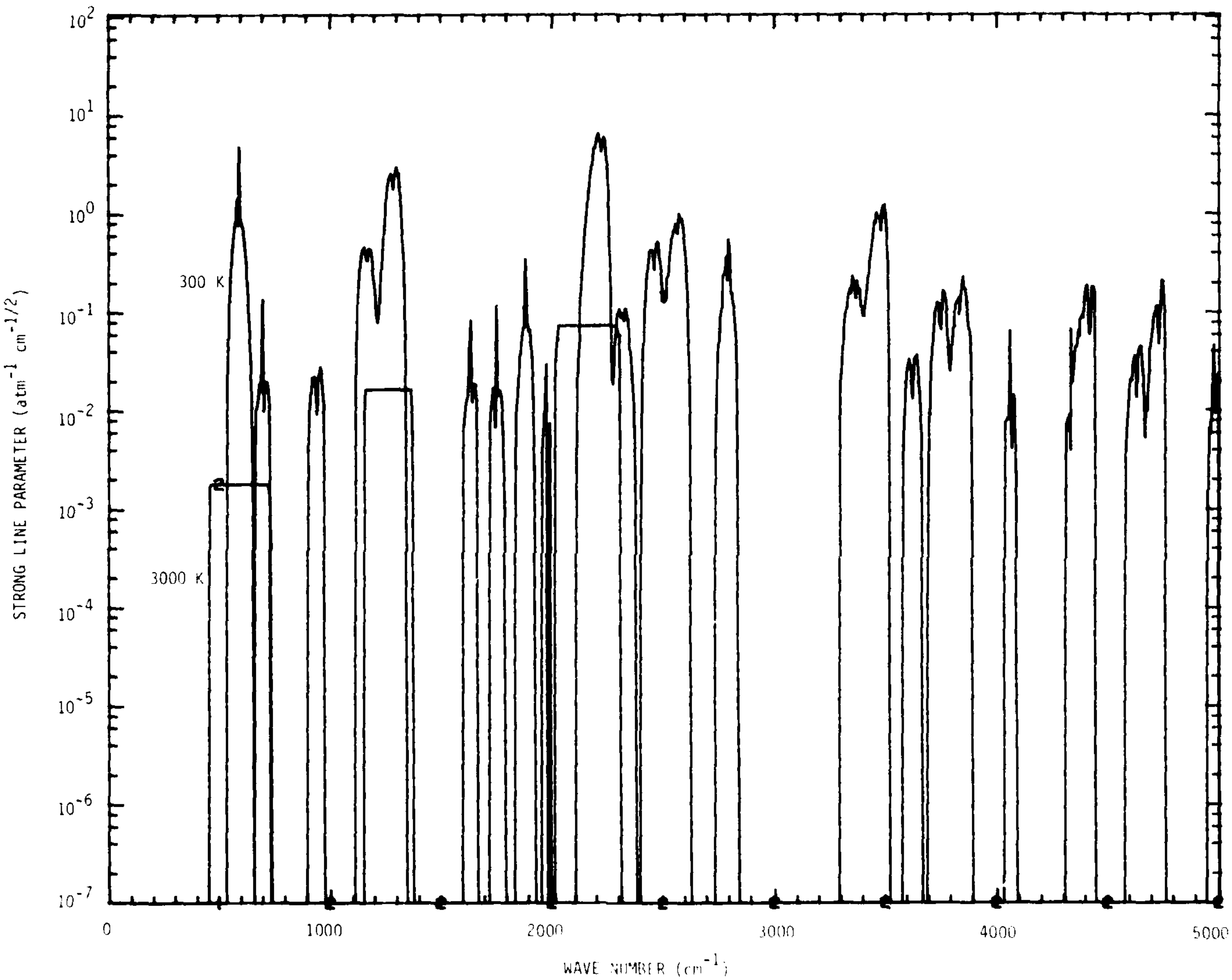

Figure 2-26. Strong line parameters for N_2O.

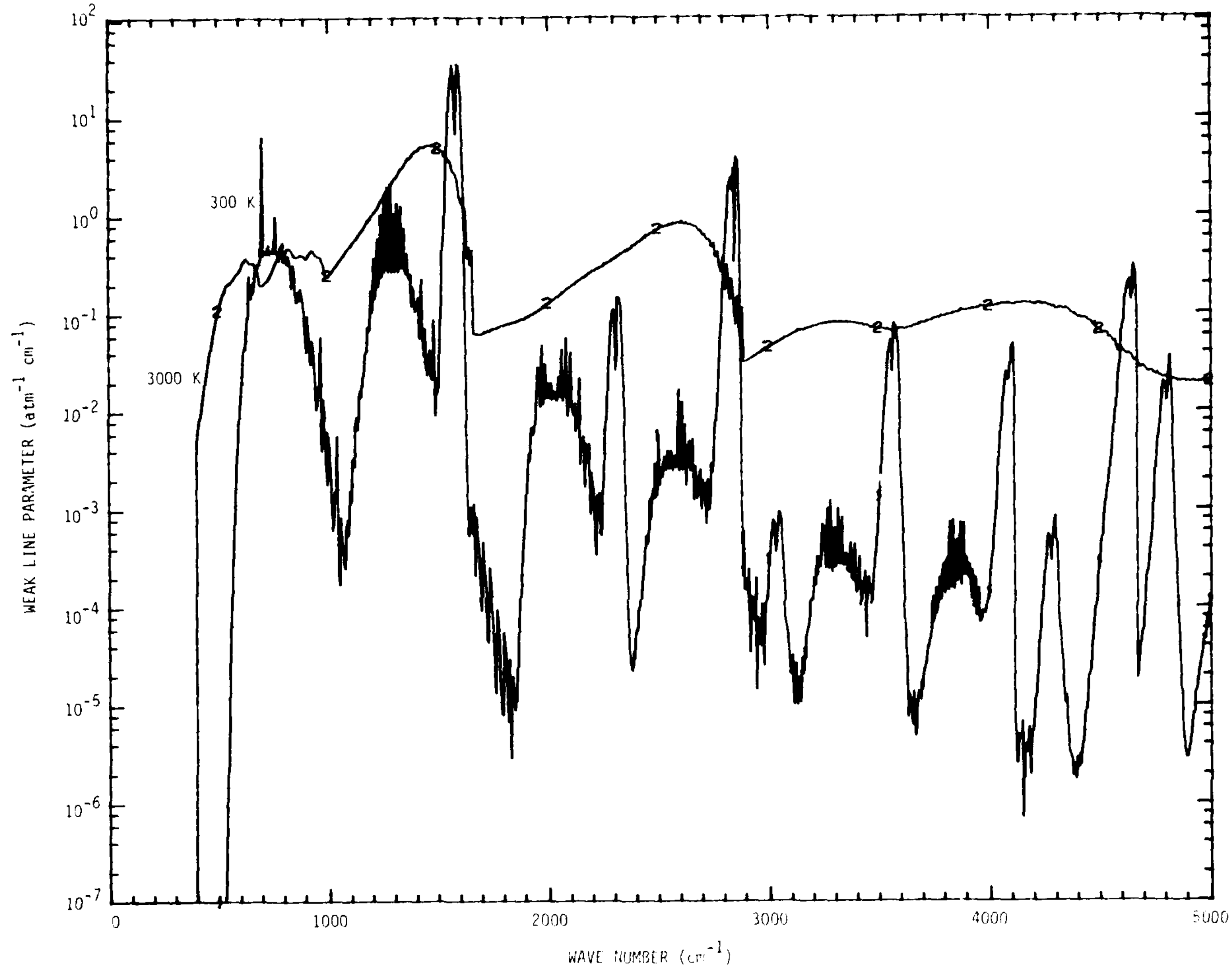

Figure 2-27. Weak line parameters for NO_2.

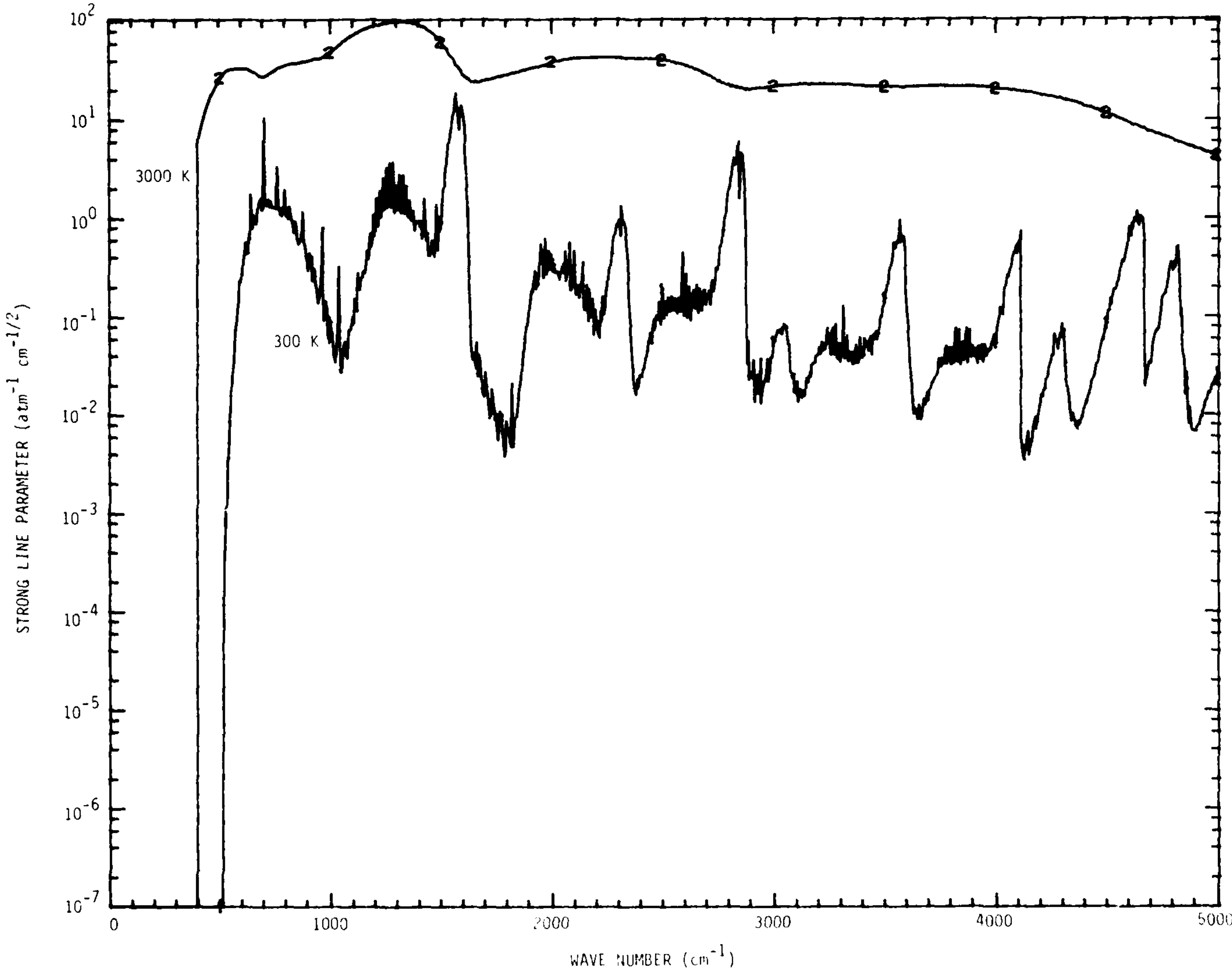

Figure 2-28. Strong line parameters for NO_2.

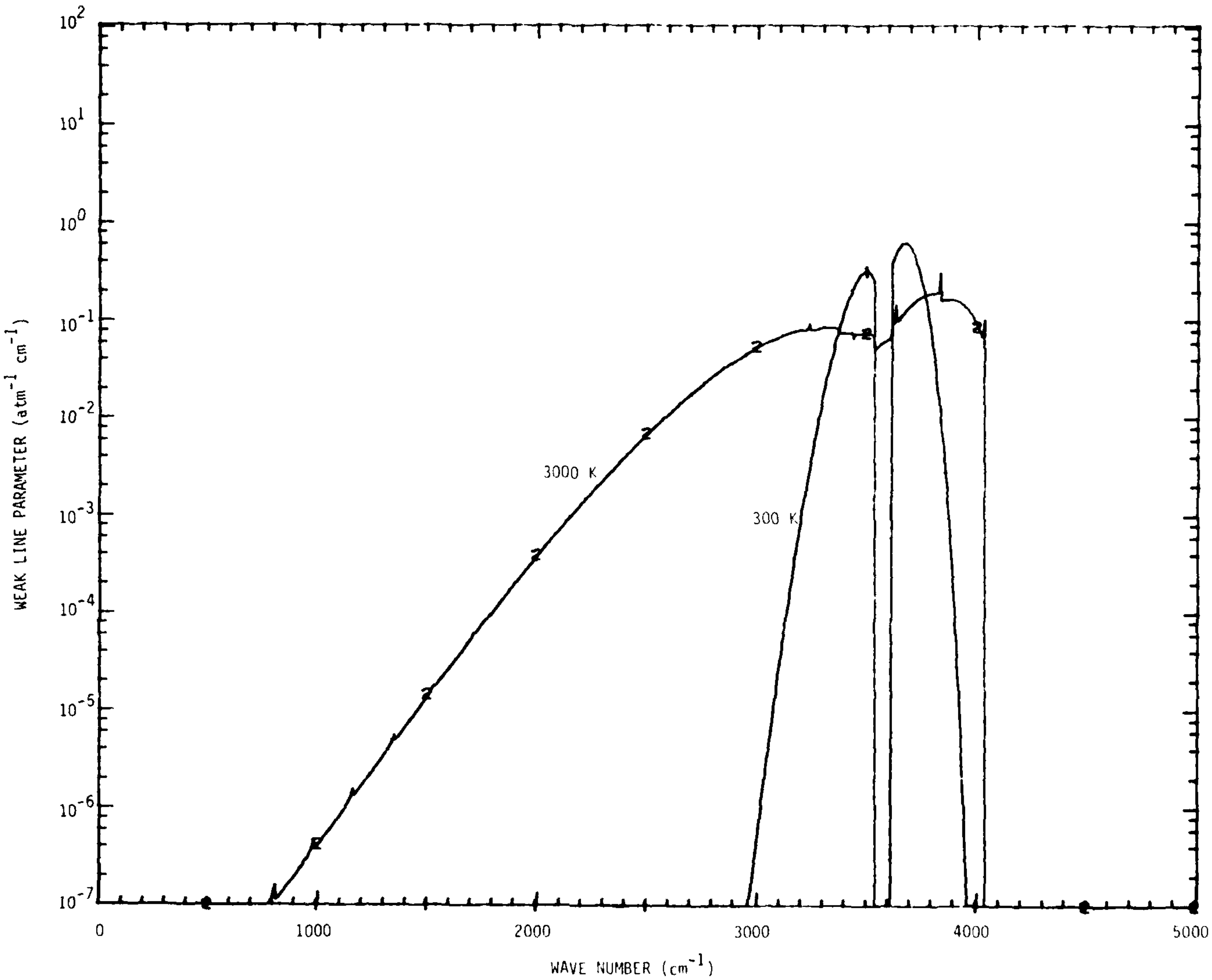

Figure 2-29. Weak line parameters for OH.

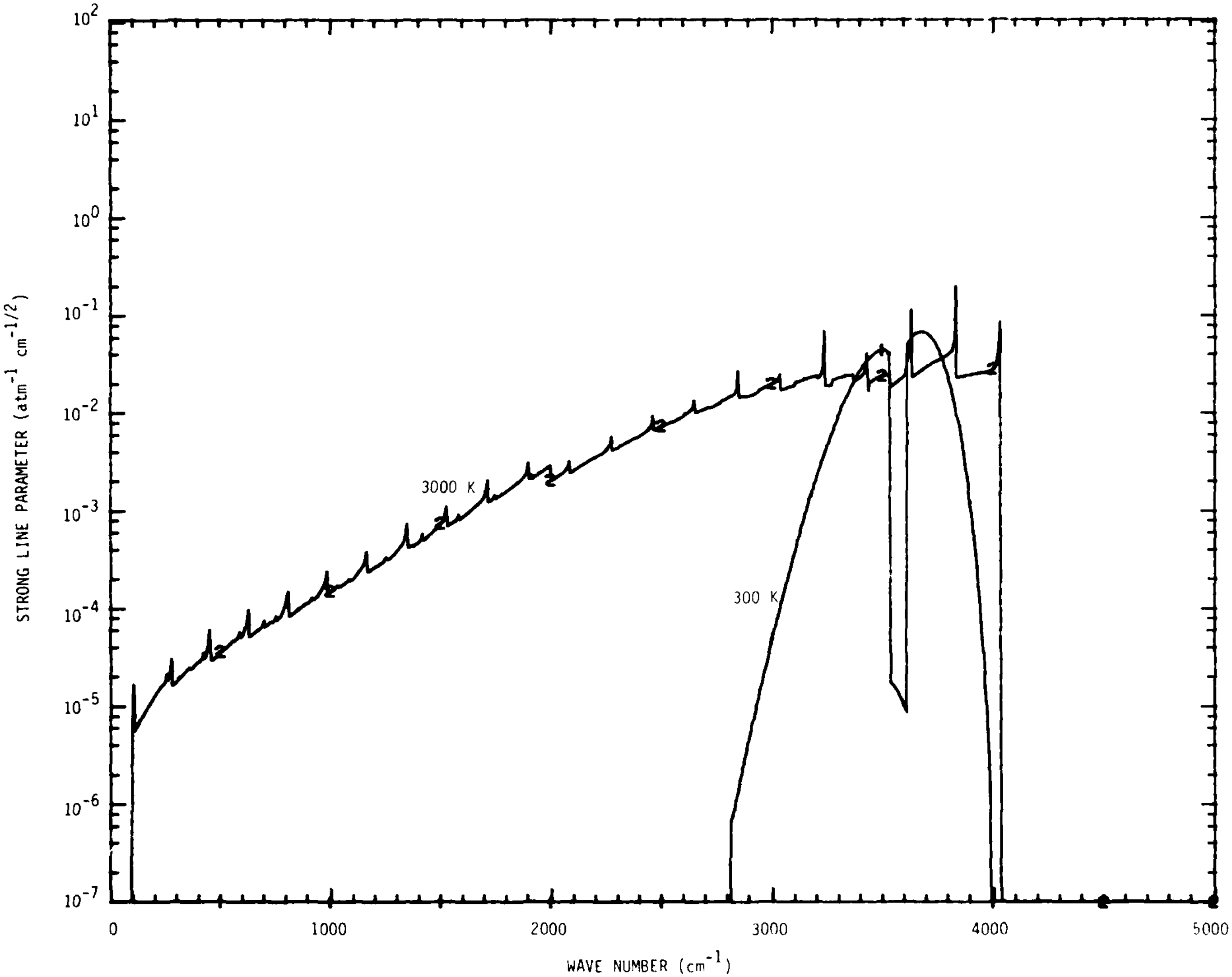

Figure 2-30. Strong line parameters for OH.

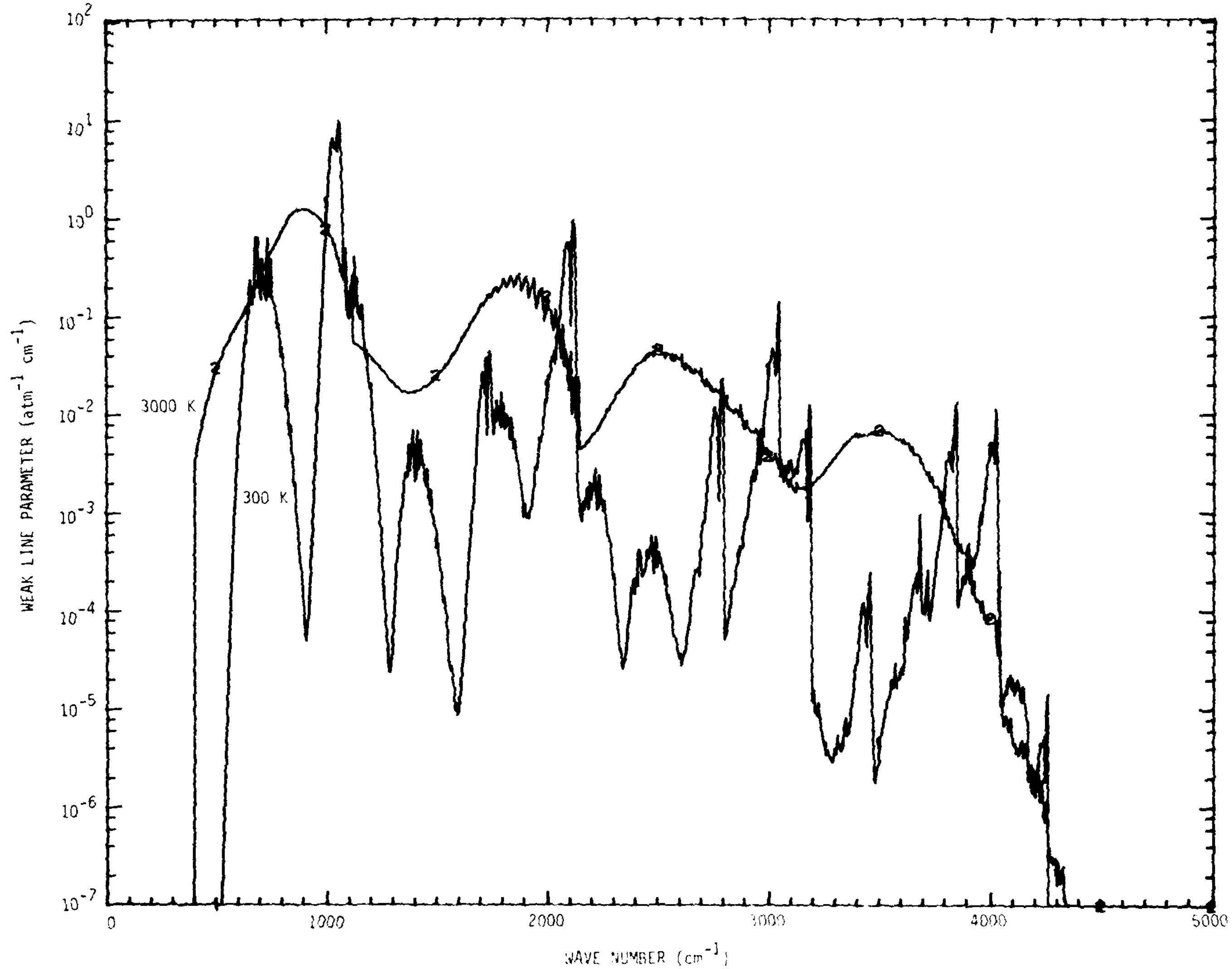

Figure 2-31. Weak line parameters for O_3.

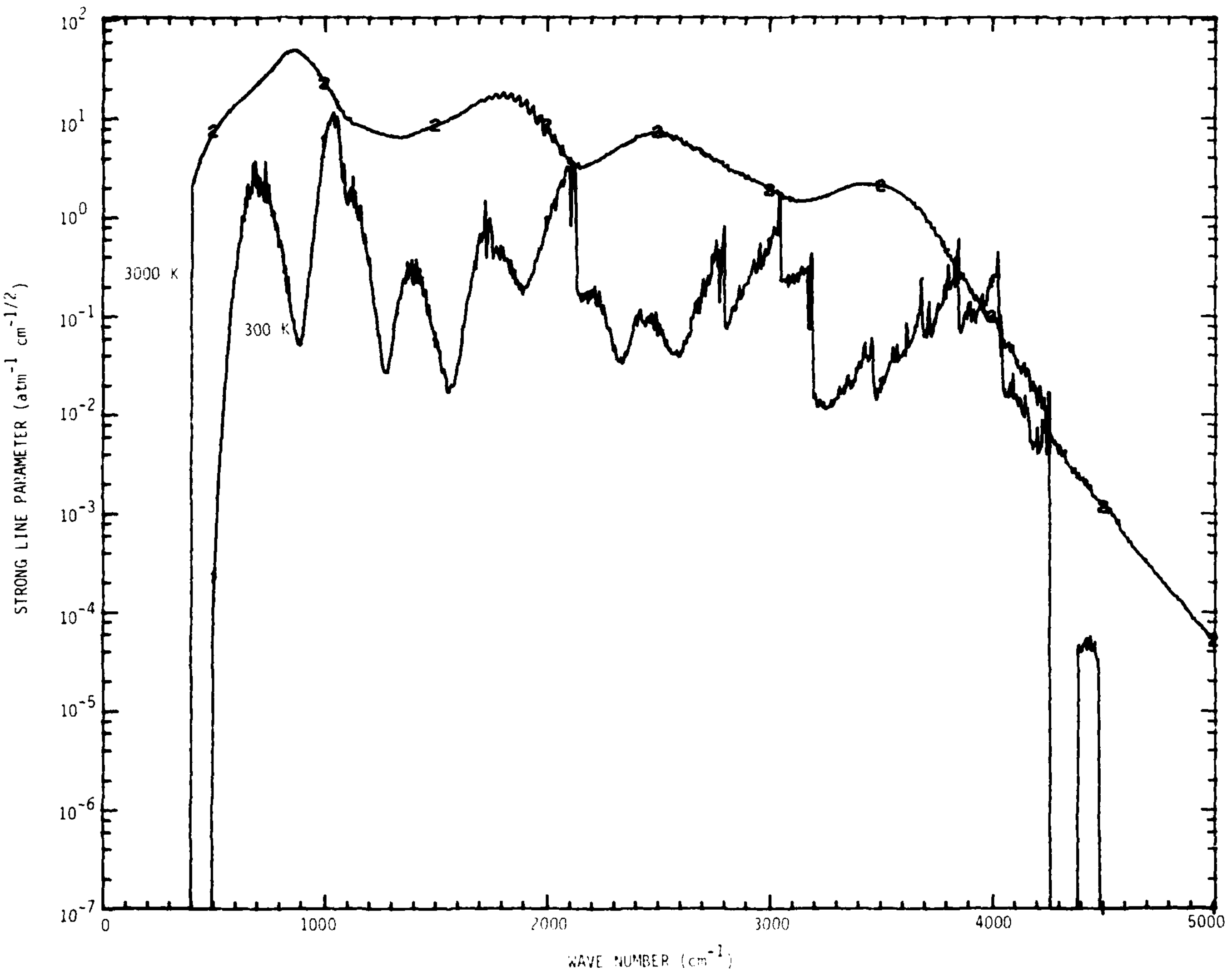

Figure 2-32. Strong line parameters for O_3.

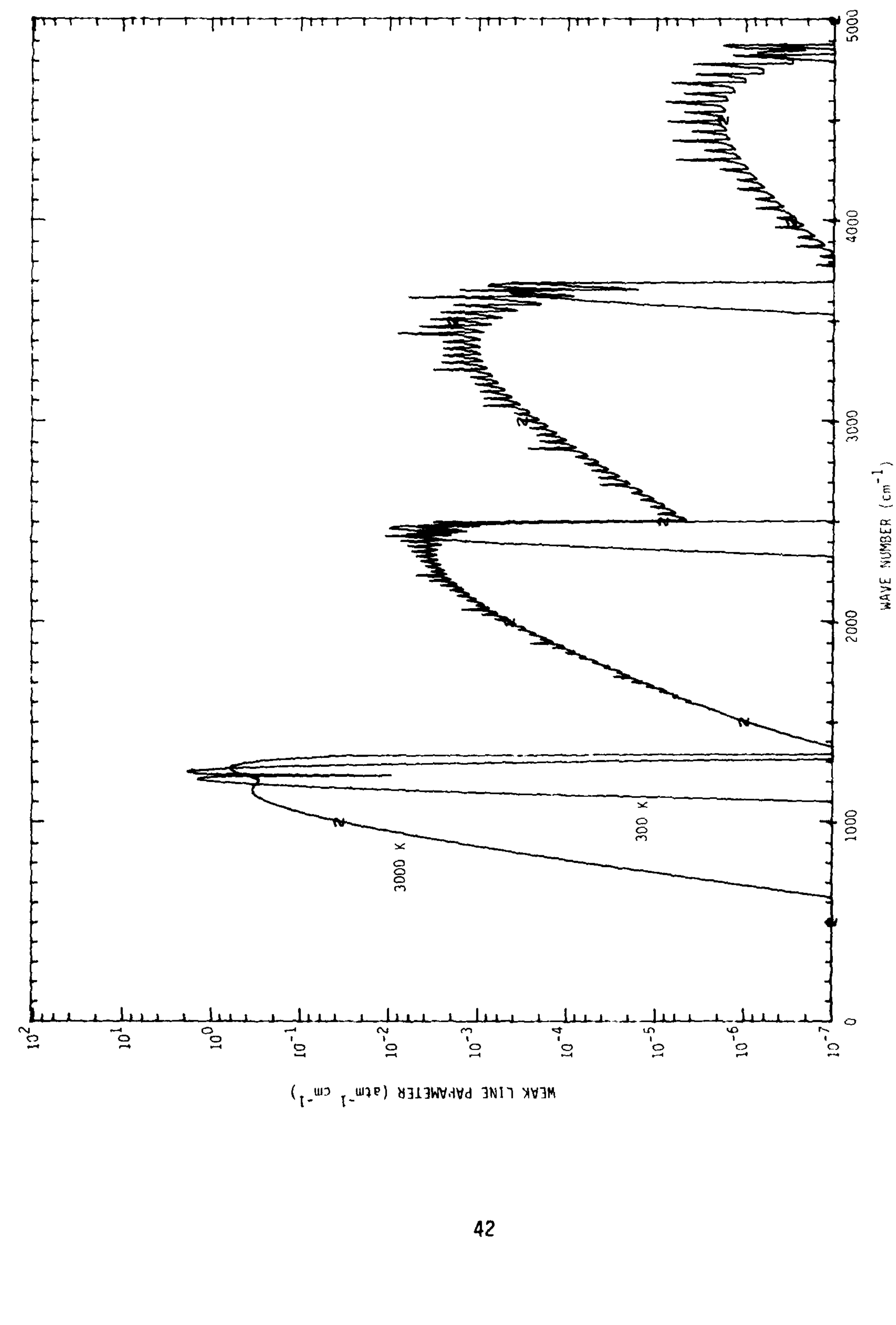

Figure 2-33. Weak line parameters for SiO.

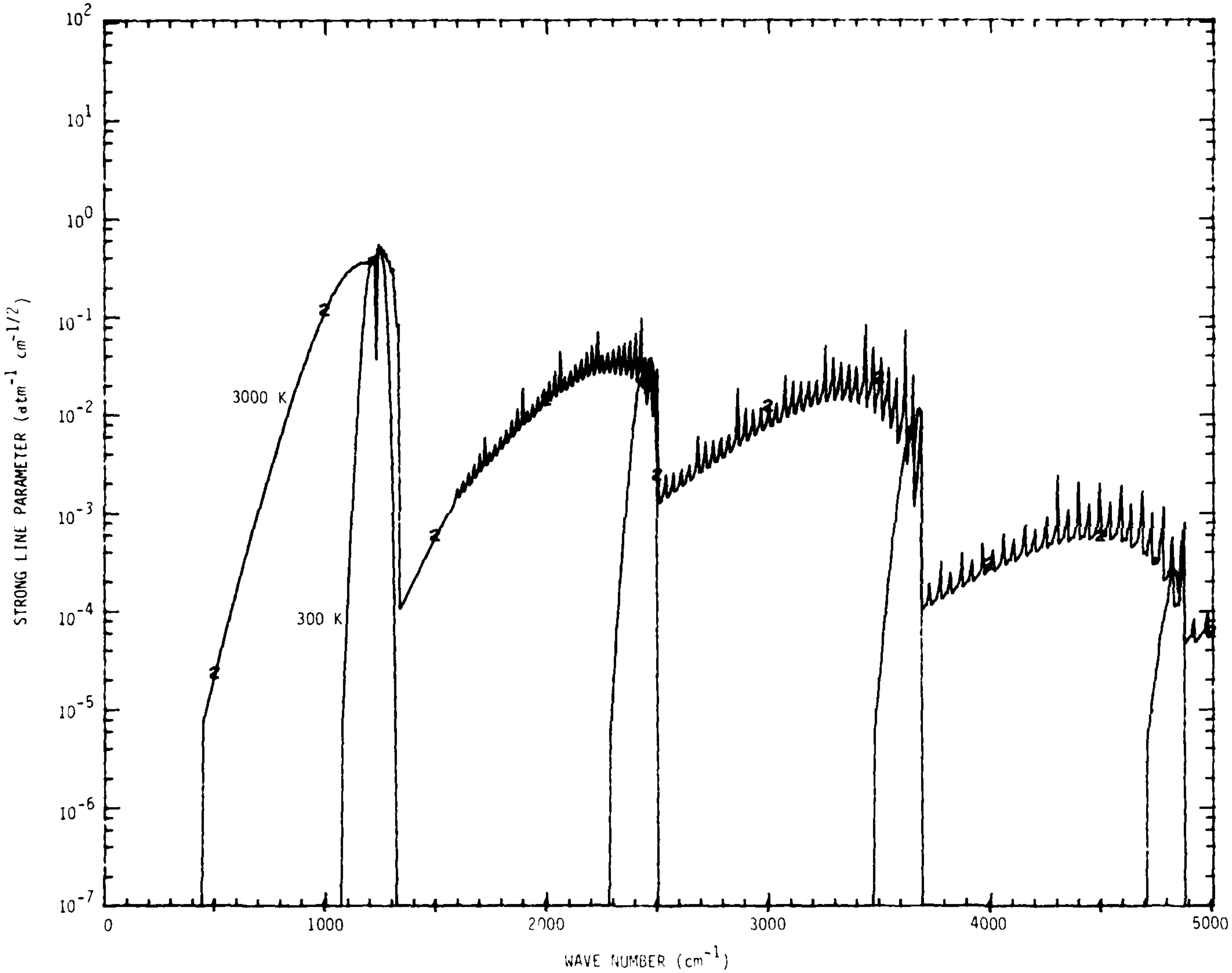

Figure 2-34. Strong l·ne parameters for SiO.

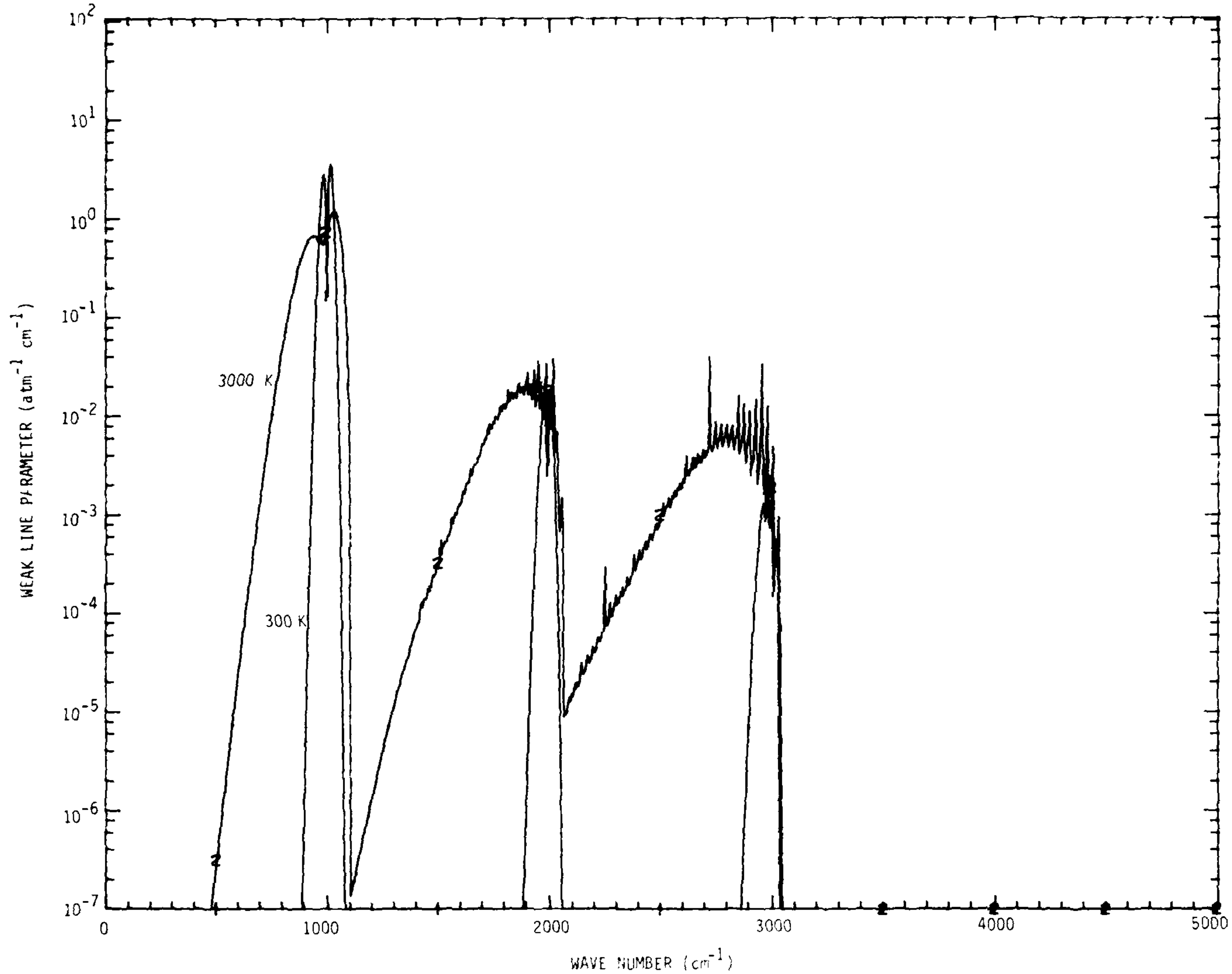

Figure 2-35. Weak line parameters for TiO.

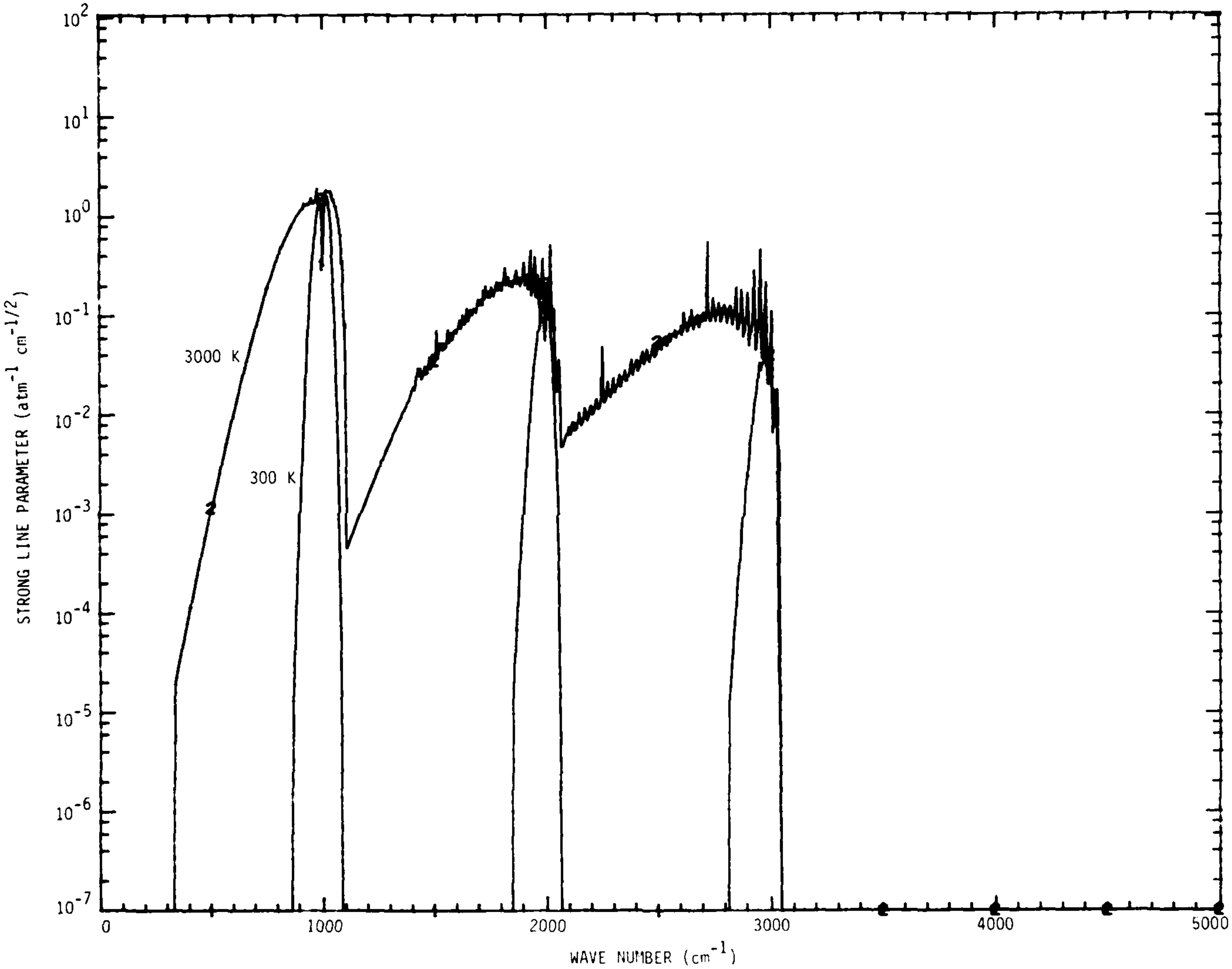

Figure 2-36. Strong line parameters for TiO.

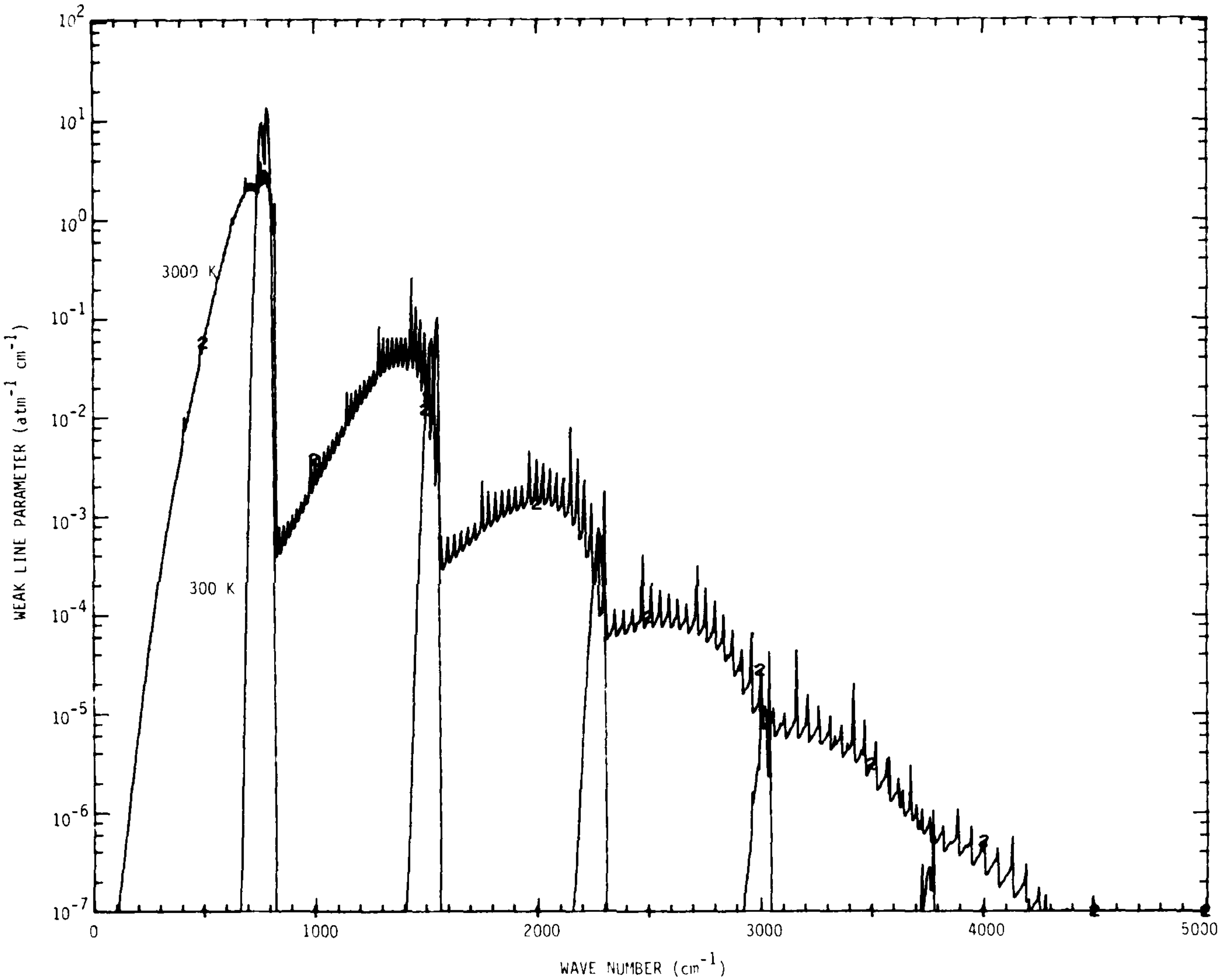

Figure 2-37. Weak line parameters for UO.

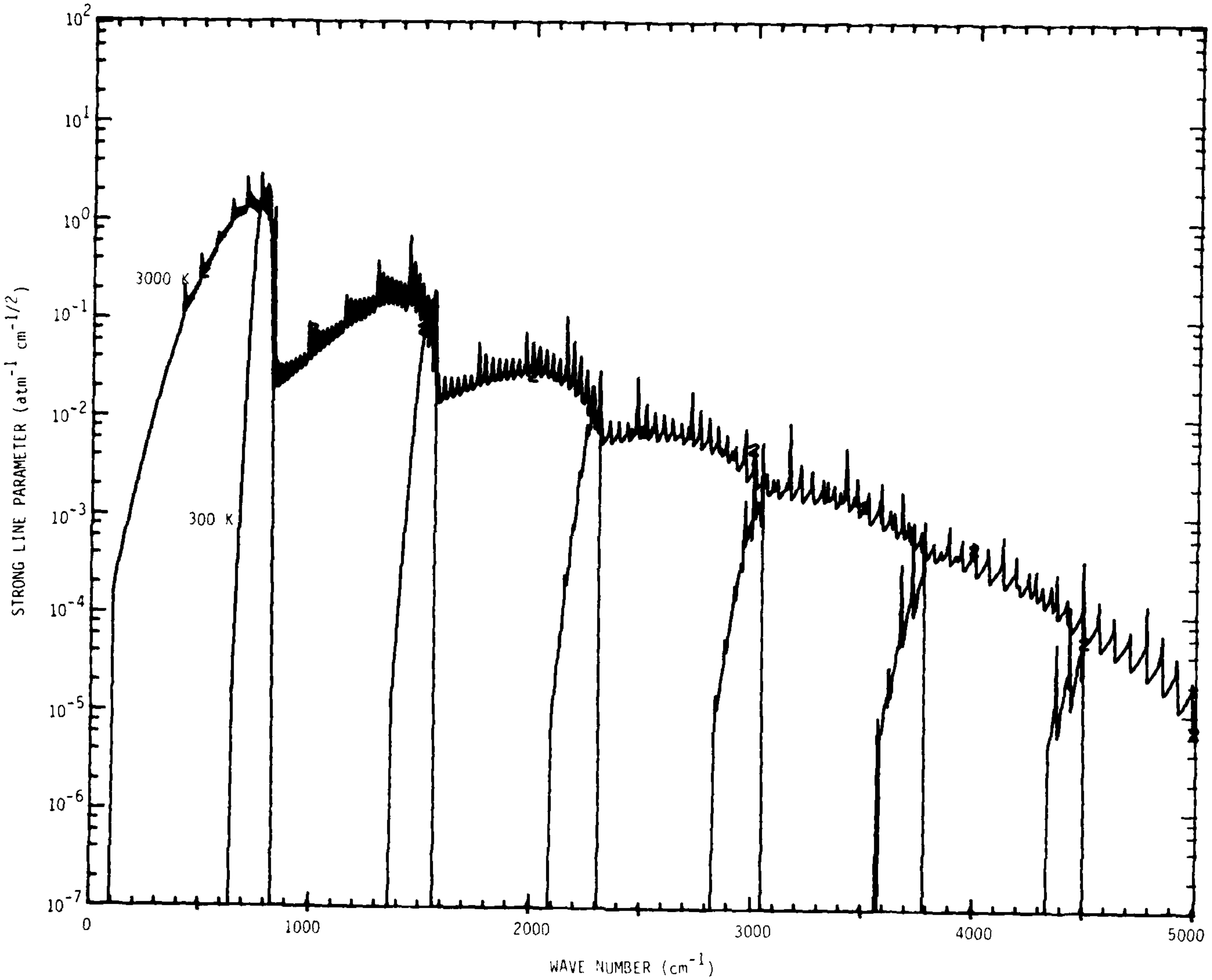

Figure 2-38. Strong line parameters for UO.

DISTRIBUTION LIST

DEPARTMENT OF DEFENSE

Assistant to the Secretary of Defense
Atomic Energy
ATTN: Executive Assistant

Defense Advanced Rsch Proj Agency
ATTN: STO, S. Zakanycz

Defense Communications Engineer Center
ATTN: Code R410, J. McLean

Defense Nuclear Agency
ATTN: RAAE, P. Lunn
4 cy ATTN: TITL

Defense Technical Information Center
12 cy ATTN: DD

Field Command
Defense Nuclear Agency
ATTN: FCPR

Field Command
Defense Nuclear Agency
Livermore Branch
ATTN: FCPRL

National Security Agency
ATTN: R-52, J. Skillman

Under Secretary of Defense for Rsch & Engrg
Department of Defense
ATTN: Strategic & Space Sys (OS)

WWMCCS System Engineering Org
ATTN: R. Crawford

DEPARTMENT OF THE ARMY

Atmospheric Sciences Laboratory
U.S. Army Electronics R&D Command
ATTN: DELAS-EO, F. Niles

BMD Advanced Technology Center
Department of the Army
ATTN: ATC-O, W. Davies
ATTN: ATC-T, M. Capps

BMD Systems Command
Department of the Army
ATTN: BMDSC-HW, R. DeKalb

Harry Diamond Laboratories
Department of the Army
ATTN: DELHD-I-TL
ATTN: DELHD-N-P, F. Wimenitz

U.S. Army Foreign Science & Tech Ctr
ATTN: DRXST-SD

U.S. Army Missile Command
ATTN: RSIC
ATTN: DRDMI-XS

U.S. Army Missile Intelligence Agency
ATTN: J. Gamble

DEPARTMENT OF THE ARMY (Continued)

U.S. Army Nuclear & Chemical Agency
ATTN: Library

U.S. Army Satellite Comm Agency
ATTN: Document Control

U.S. Army TRADOC Sys Analysis Actvy
ATTN: ATAA-PL

DEPARTMENT OF THE NAVY

Naval Electronic Systems Command
ATTN: Code 501A
ATTN: PME 117-20

Naval Intelligence Support Ctr
ATTN: Document Control

Naval Ocean Systems Center
ATTN: Code 532

Naval Postgraduate School
ATTN: Code 1424, Library

Naval Research Laboratory
ATTN: Code 4780, P. Palmadesso
ATTN: Code 2627
ATTN: Code 4780, S. Ossakow
ATTN: Code 4709, W. Ali
ATTN: Code 4700, T. Coffey
ATTN: Code 4701, J. Brown

Naval Surface Weapons Center
ATTN: Code X211

Strategic Systems Project Office
Department of the Navy
ATTN: NSP-2722, F. Wimberly
ATTN: NSSP-2722, M. Meserole

DEPARTMENT OF THE AIR FORCE

Air Force Geophysics Laboratory
ATTN: SULL
ATTN: LKB, K. Champion
ATTN: OPR, A. Stair
ATTN: OPR, H. Gardiner

Air Force Systems Command
ATTN: Technical Library

Air Force Technical Applications Ctr
ATTN: TFR, C. Meneely
ATTN: Technical Library

Air Force Weapons Laboratory
Air Force Systems Command
ATTN: SUL
ATTN: NTYC

Air University Library
Department of the Air Force
ATTN: AUL-LSE

DEPARTMENT OF THE AIR FORCE (Continued)

Ballistic Missile Office
Air Force Systems Command
ATTN: PM
ATTN: SYDT
ATTN: SYC

Deputy Chief of Staff
Research, Development, & Acq
Department of the Air Force
ATTN: AFRDS

Headquarters Space Division
Air Force Systems Command
ATTN: SKA, M. Clavin
ATTN: SKX

Headquarters Space Division
Air Force Systems Command
ATTN: SZJ, P. Kelley

Rome Air Development Center
Air Force Systems Command
ATTN: OCSA, J. Simons
ATTN: TSLD
ATTN: OCS, V. Coyne

Strategic Air Command
Department of the Air Force
ATTN: NRT
ATTN: XPFS

DEPARTMENT OF ENERGY

Department of Energy
ATTN: OMA

OTHER GOVERNMENT AGENCIES

Department of Commerce
National Oceanic & Atomospheric Admin
ATTN: F. Fehsenfeld

Institute for Telecommunications Sciences
National Telecommunications & Info Admin
ATTN: W. Utlaut
ATTN: G. Falcon

DEPARTMENT OF DEFENSE CONTRACTORS

Aerojet Electro-Systems Co
ATTN: J. Graham

Aerospace Corp
ATTN: I. Garfunkel
ATTN: N. Stockwell
ATTN: J. Reinheimer
ATTN: N. Cohen
ATTN: J. Straus
ATTN: V. Josephson

Berkeley Research Associates, Inc
ATTN: J. Workman

ESL, Inc
ATTN: J. Marshall

General Electric Co
ATTN: M. Bortner

DEPARTMENT OF DEFENSE CONTRACTORS (Continued)

General Research Corp
ATTN: J. Garbarino
ATTN: J. Ise, Jr

Jamieson Science & Engineering
ATTN: J. Jamieson

Kaman Sciences Corp
ATTN: P. Tracy
ATTN: D. Perio
ATTN: N. Beauchamp

Kaman Tempo
ATTN: W. Knapp
ATTN: DASIAC
ATTN: J. Jordano
ATTN: K. Schwartz
4 cy ATTN: T. Stephens
4 cy ATTN: A. Klein

Lockheed Missiles & Space Co, Inc
ATTN: D. Divis

Lockheed Missiles & Space Co, Inc
ATTN: M. Walt

M.I.T. Lincoln Lab
ATTN: D. Towle

McDonnell Douglas Corp
ATTN: R. Halprin
ATTN: H. Spitzer

Mission Research Corp
ATTN: R. Bogusch
ATTN: D. Archer
ATTN: R. Kilb
ATTN: D. Sappenfield
ATTN: R. Hendrick
ATTN: M. Scheibe
ATTN: F. Fajen

Nichols Research Corp, Inc
ATTN: N. Byrn

Pacific-Sierra Research Corp
ATTN: H. Brode

Photometrics, Inc
ATTN: I. Kofsky

Physical Research, Inc
ATTN: R. Deliberis

University of the Commonwealth, Pittsburgh
ATTN: F. Kaufman

R & D Associates
ATTN: B. Gabbard
ATTN: R. Turco
ATTN: F. Gilmore
ATTN: R. Lelevier
ATTN: P. Haas

R & D Associates
ATTN: B. Yoon

Rand Corp
ATTN: C. Crain

DEPARTMENT OF DEFENSE CONTRACTORS (Continued)

Science Applications, Inc
ATTN: D. Hamlin

Science Applications, Inc
ATTN: W. Mendes

SRI International
ATTN: W. Jaye
ATTN: W. Chesnut

DEPARTMENT OF DEFENSE CONTRACTORS (Continued)

Teledyne Brown Engineering
ATTN: J. Cato
ATTN: Technical Library
ATTN: G. Harney
ATTN: J. Ford

Visidyne, Inc
ATTN: H. Smith
ATTN: C. Humphrey
ATTN: J. Carpenter